

*Physical Chemistry Chemical Physics*

**Electronic Supporting Information**

**An Overview of Performance of COSMO-RS Approach in Predicting  
Activity Coefficients of Molecular Solutes in Ionic Liquids and Derived  
Properties at Infinite Dilution**

Kamil Padászyński<sup>1</sup>

*Department of Physical Chemistry, Faculty of Chemistry  
Warsaw University of Technology, Noakowskiego 3, 00-664 Warsaw, Poland*

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<sup>1</sup>To whom correspondence should be sent: kpaduszynski@ch.pw.edu.pl; Phone: +48 22 234 56 40.

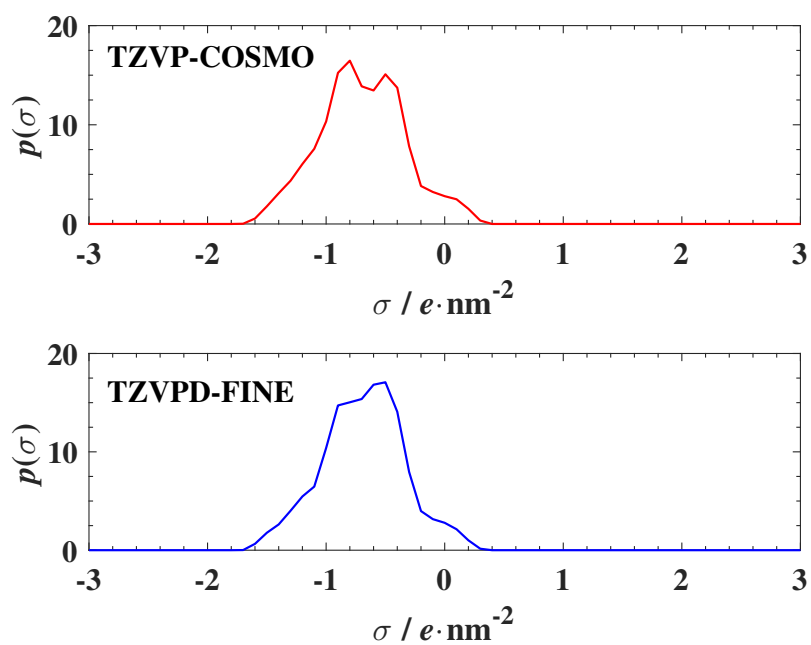
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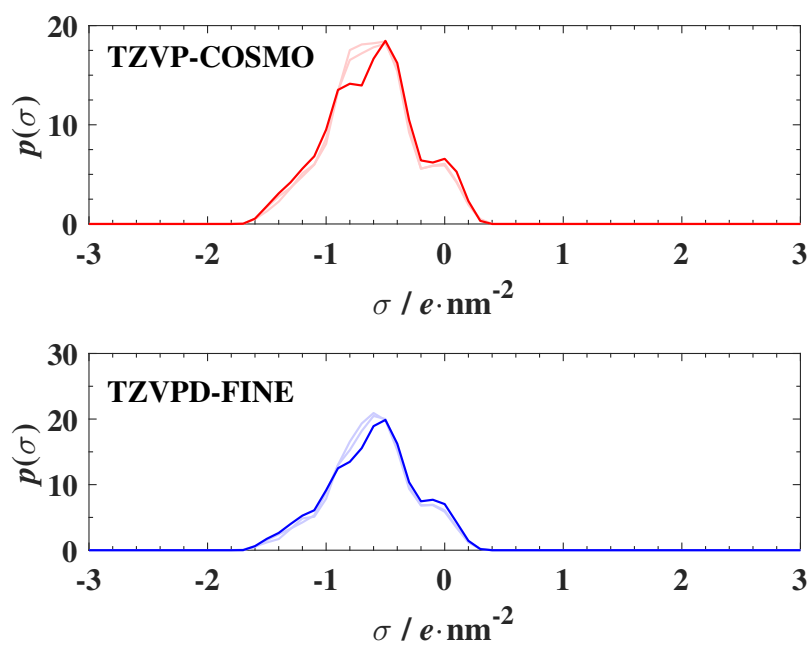
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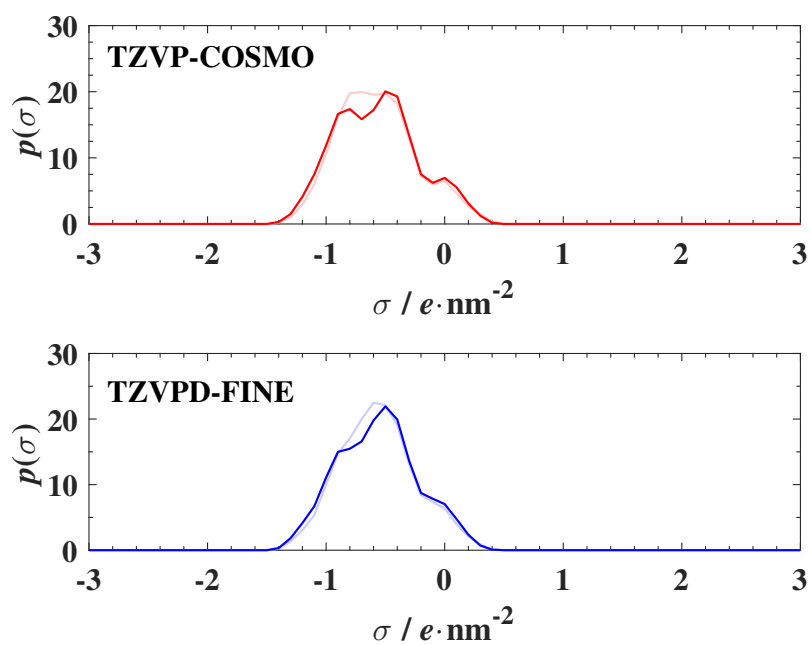
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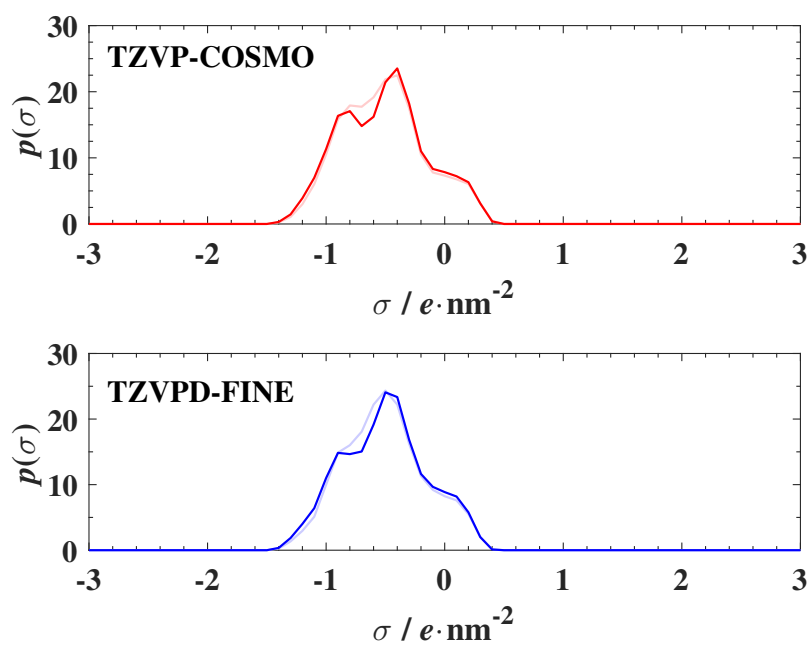
**Figure S1.**  $\sigma$ -profiles of IM-1,1 cation (abbreviations explained in the supplied Microsoft Excel spreadsheet, Table S1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



**Figure S2.**  $\sigma$ -profiles of IM-2,1 cation (abbreviations explained in the supplied Microsoft Excel spreadsheet, Table S1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).

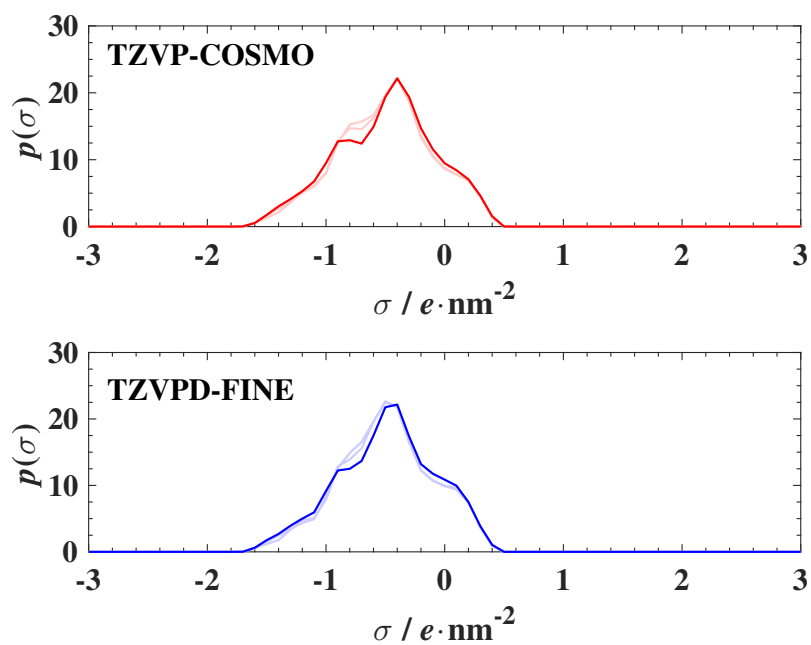


**Figure S3.**  $\sigma$ -profiles of IM-2, 1, 1 cation (abbreviations explained in the supplied Microsoft Excel spreadsheet, Table S1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).

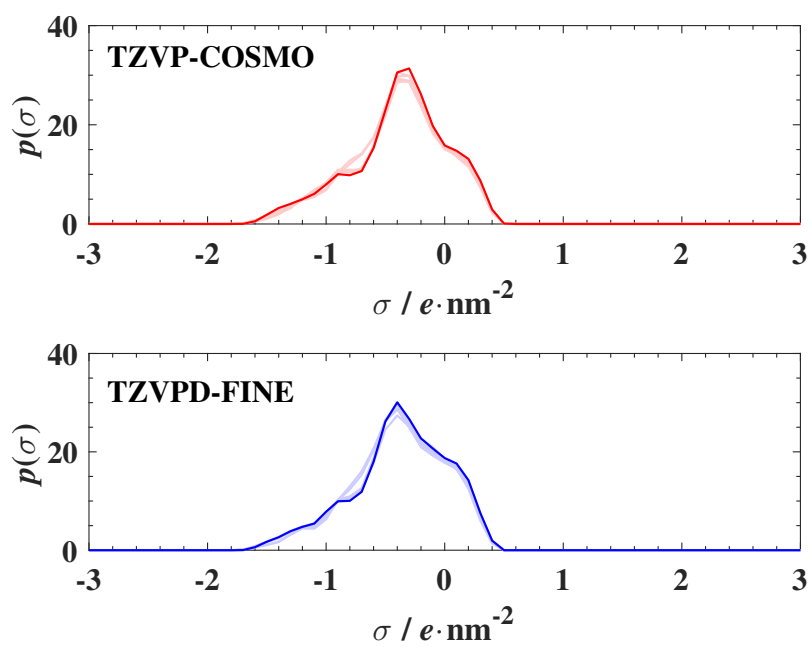


**Figure S4.**  $\sigma$ -profiles of IM-3, 1, 1 cation (abbreviations explained in the supplied Microsoft Excel spreadsheet, Table S1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).

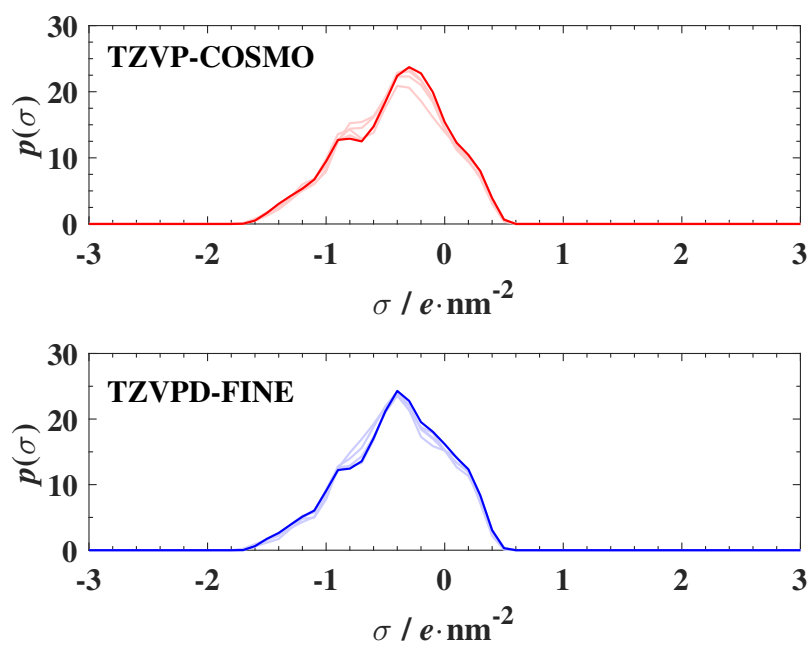




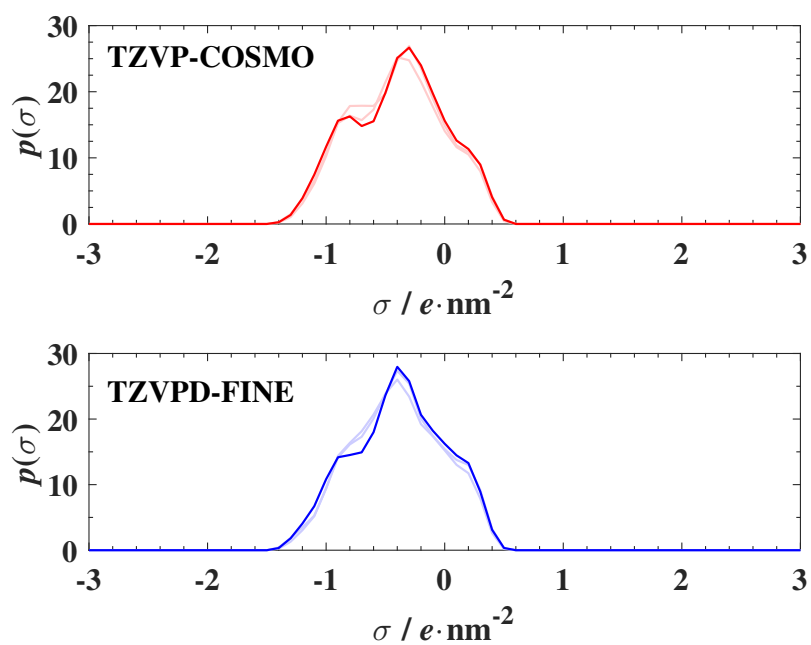
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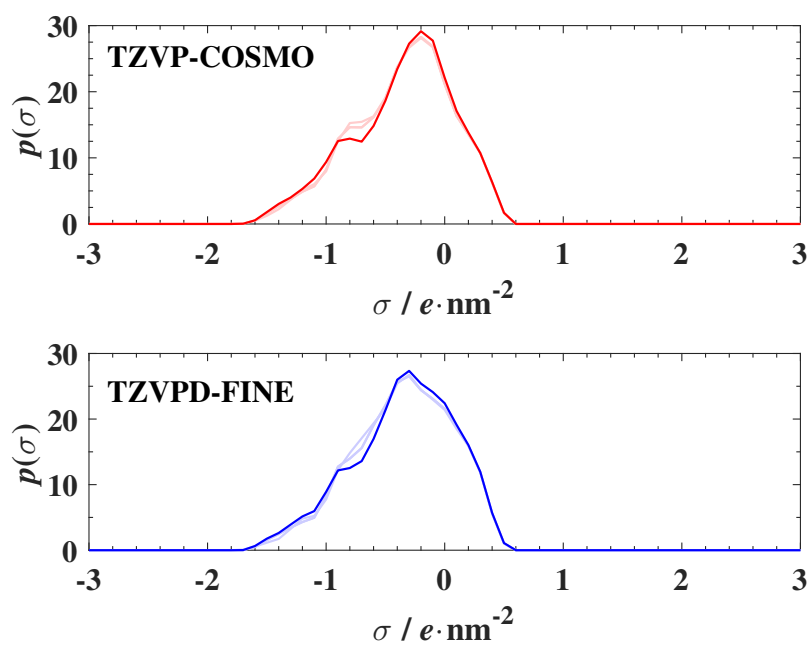
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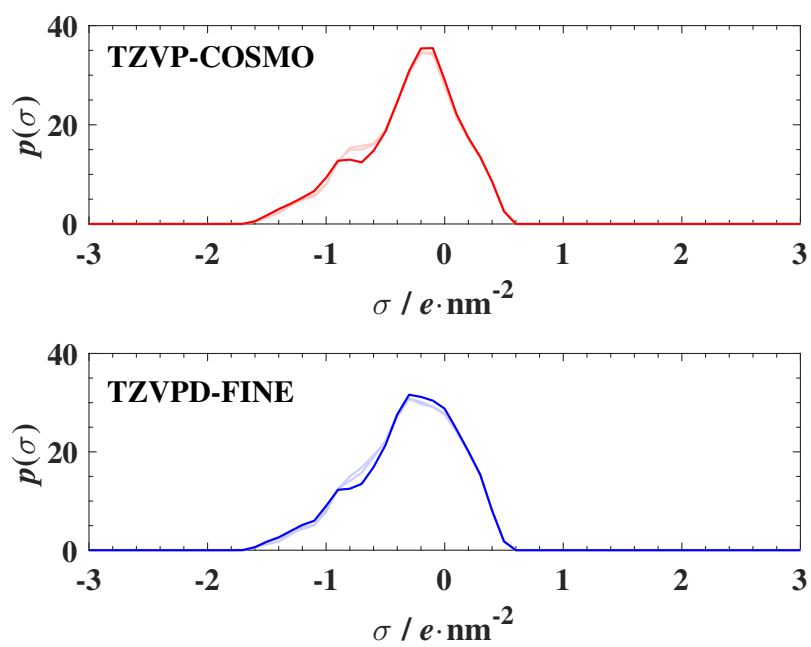
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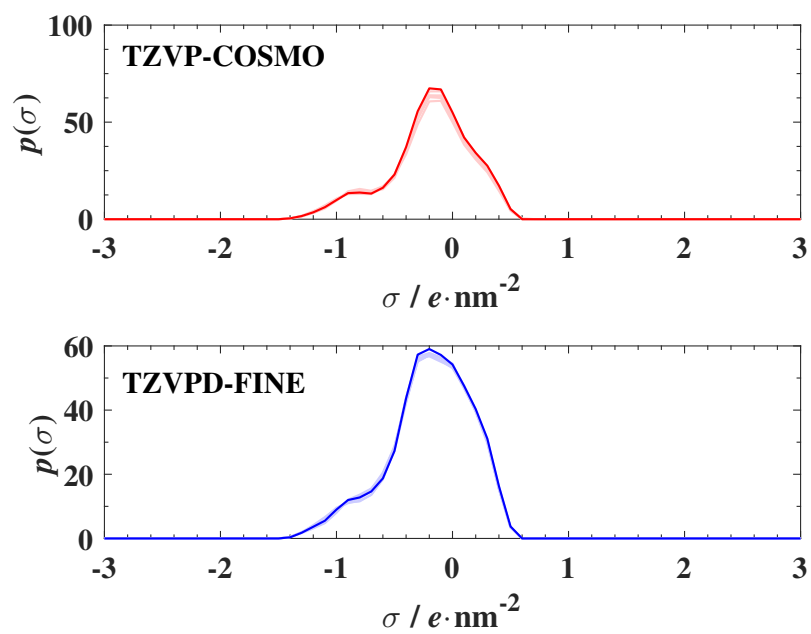
**Figure S8.**  $\sigma$ -profiles of IM-6, 1, 1 cation (abbreviations explained in the supplied Microsoft Excel spreadsheet, Table S1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



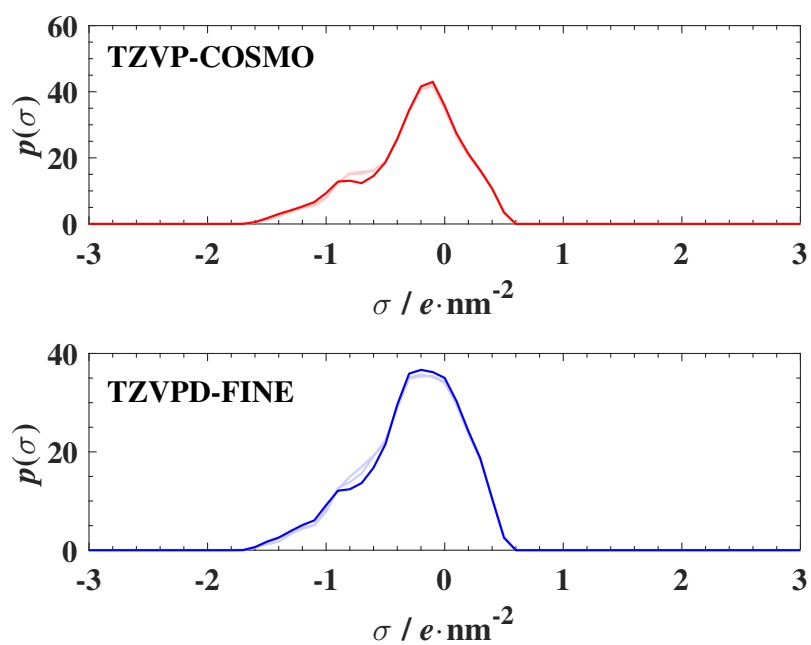
**Figure S9.**  $\sigma$ -profiles of IM-8,1 cation (abbreviations explained in the supplied Microsoft Excel spreadsheet, Table S1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



**Figure S10.**  $\sigma$ -profiles of IM-10,1 cation (abbreviations explained in the supplied Microsoft Excel spreadsheet, Table S1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).

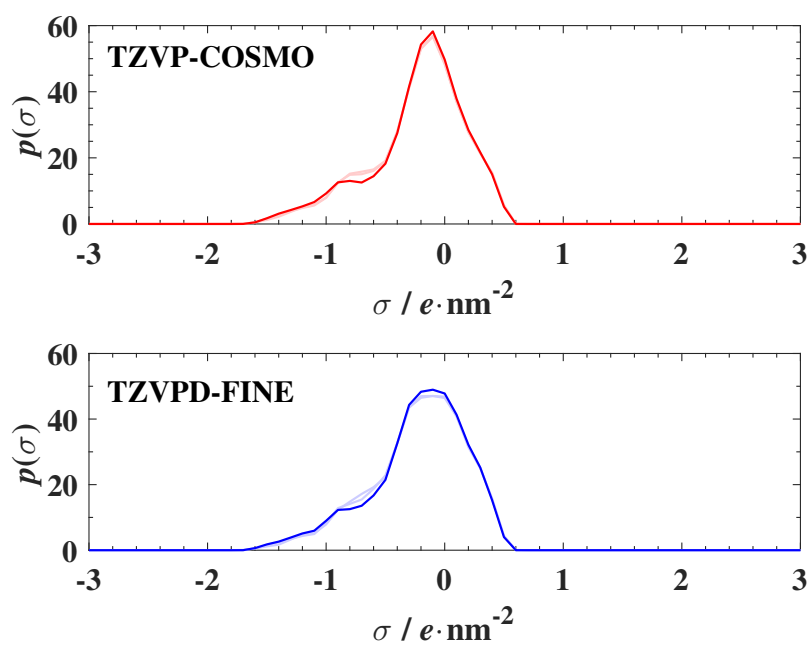


**Figure S11.**  $\sigma$ -profiles of IM-10,10,1 cation (abbreviations explained in the supplied Microsoft Excel spreadsheet, Table S1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).

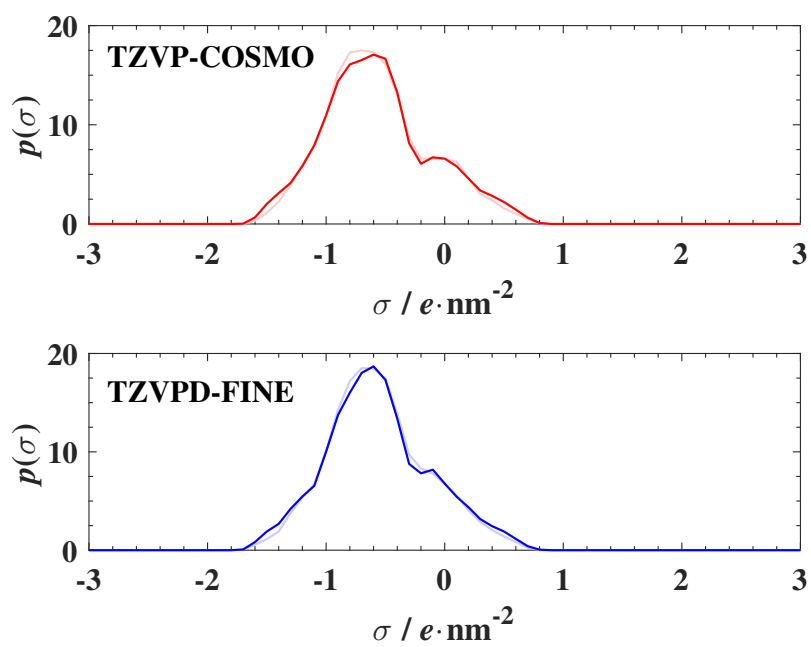


**Figure S12.**  $\sigma$ -profiles of IM-12,1 cation (abbreviations explained in the supplied Microsoft Excel spreadsheet, Table S1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).

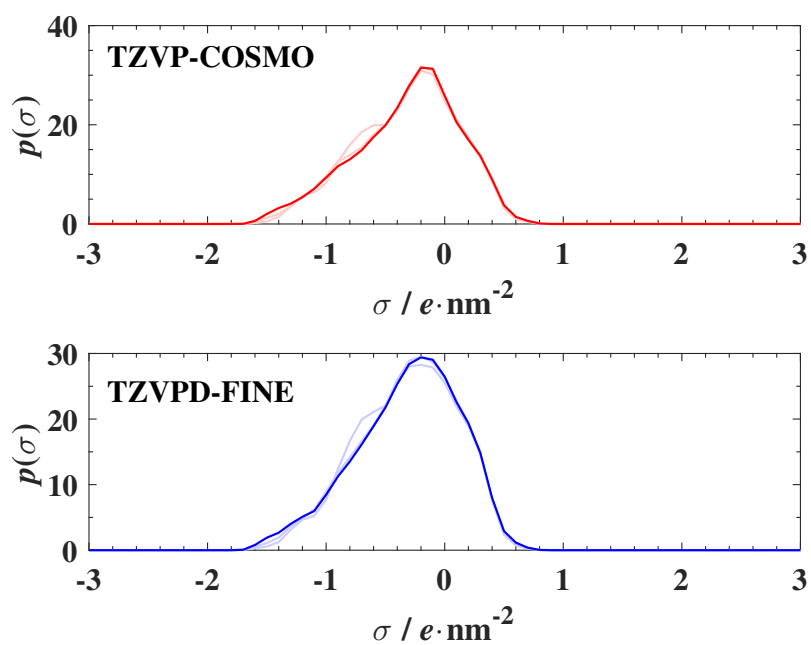




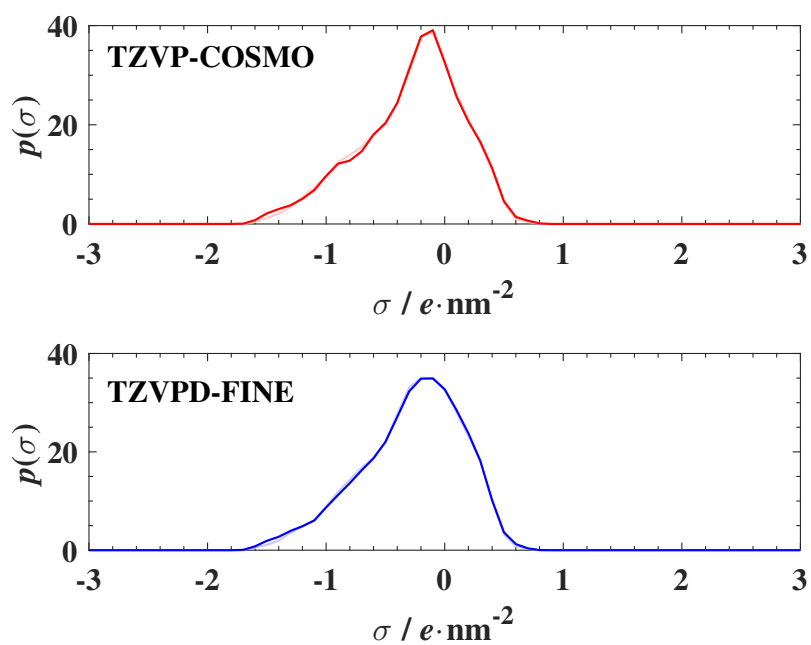
**Figure S13.**  $\sigma$ -profiles of IM-16,1 cation (abbreviations explained in the supplied Microsoft Excel spreadsheet, Table S1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



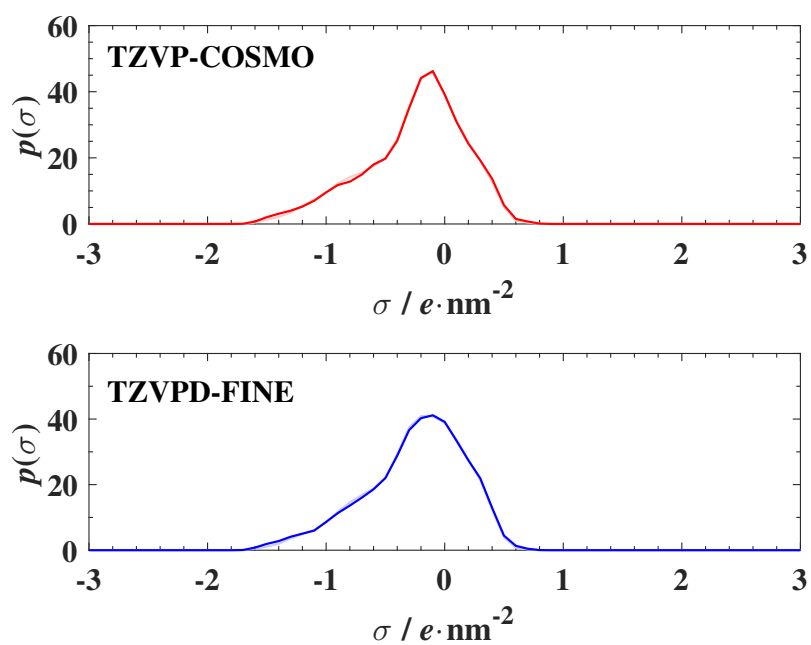
**Figure S14.**  $\sigma$ -profiles of IM-A,1 cation (abbreviations explained in the supplied Microsoft Excel spreadsheet, Table S1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



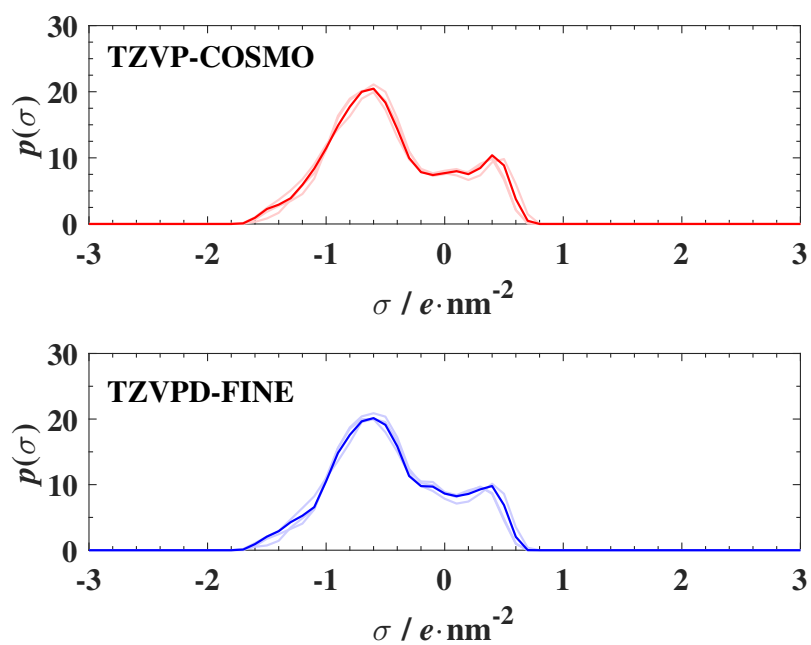
**Figure S15.**  $\sigma$ -profiles of IM-A,8 cation (abbreviations explained in the supplied Microsoft Excel spreadsheet, Table S1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



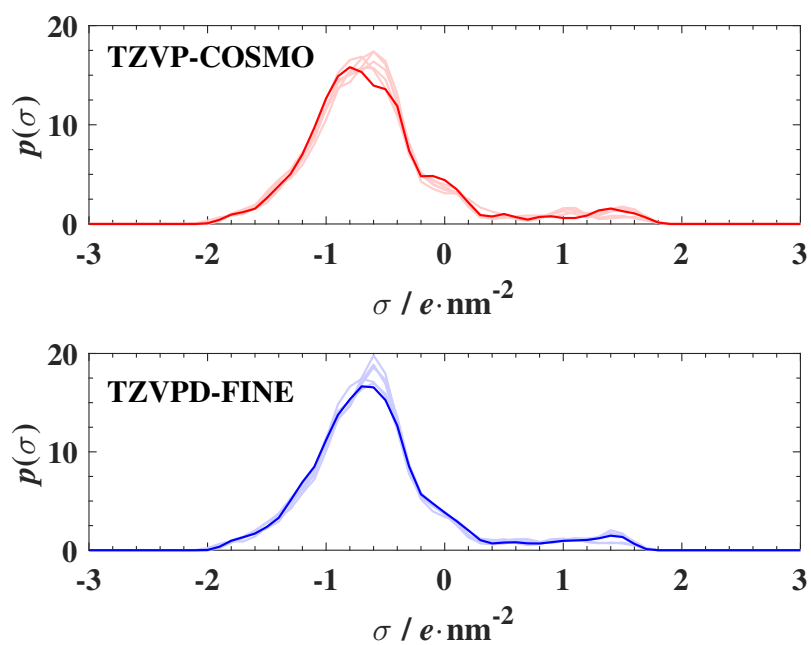
**Figure S16.**  $\sigma$ -profiles of IM-A, **10** cation (abbreviations explained in the supplied Microsoft Excel spreadsheet, Table S1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



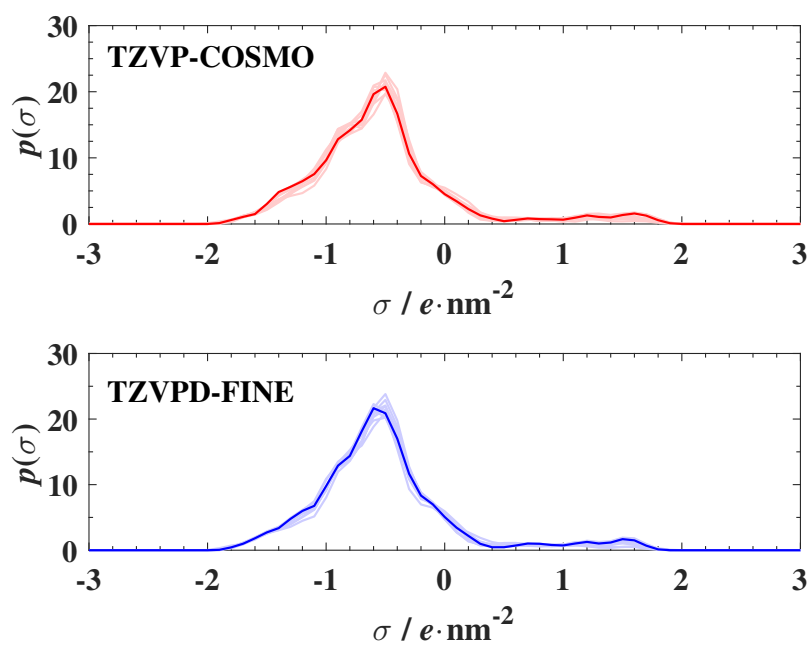
**Figure S17.**  $\sigma$ -profiles of IM-A, 12 cation (abbreviations explained in the supplied Microsoft Excel spreadsheet, Table S1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



**Figure S18.**  $\sigma$ -profiles of IM-1PH, 1 cation (abbreviations explained in the supplied Microsoft Excel spreadsheet, Table S1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).

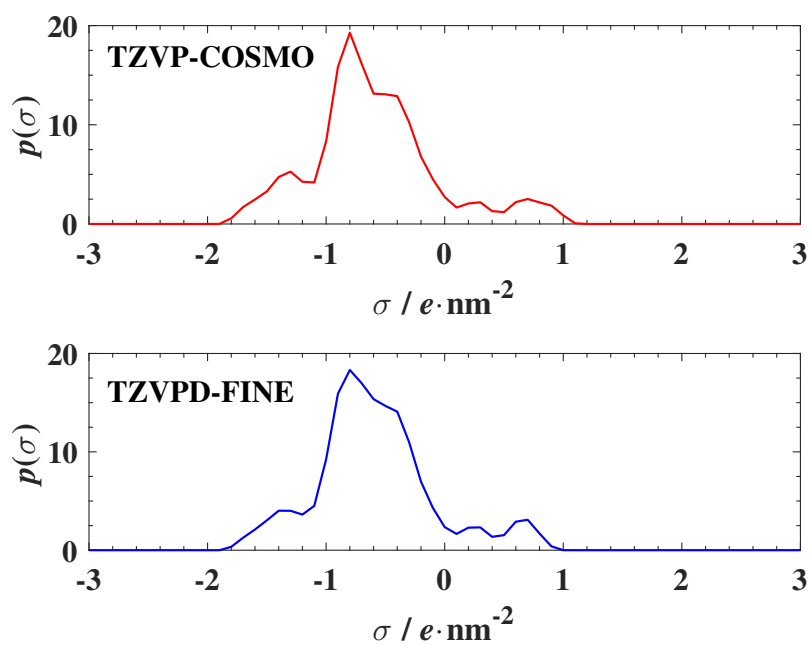


**Figure S19.**  $\sigma$ -profiles of IM-20H, 1 cation (abbreviations explained in the supplied Microsoft Excel spreadsheet, Table S1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).

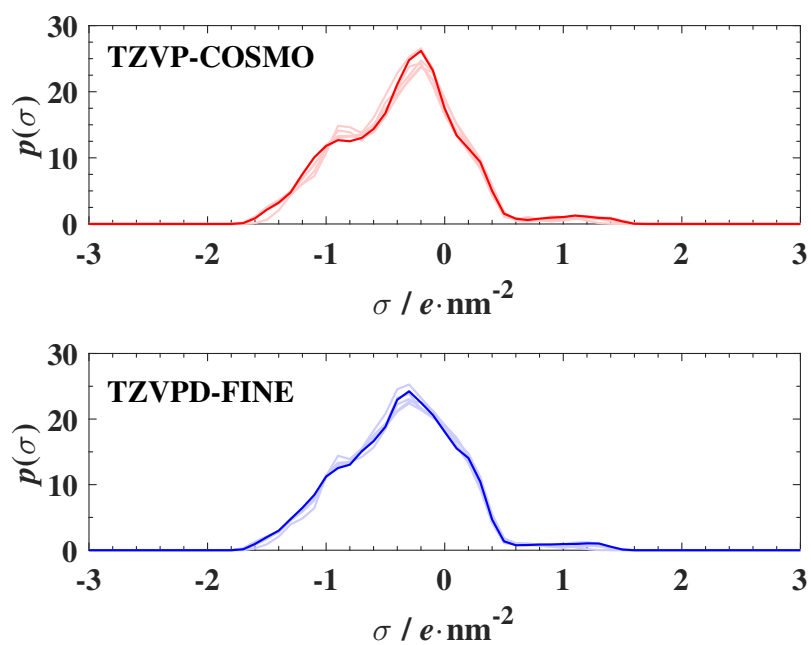


**Figure S20.**  $\sigma$ -profiles of IM-30H, 1 cation (abbreviations explained in the supplied Microsoft Excel spreadsheet, Table S1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).

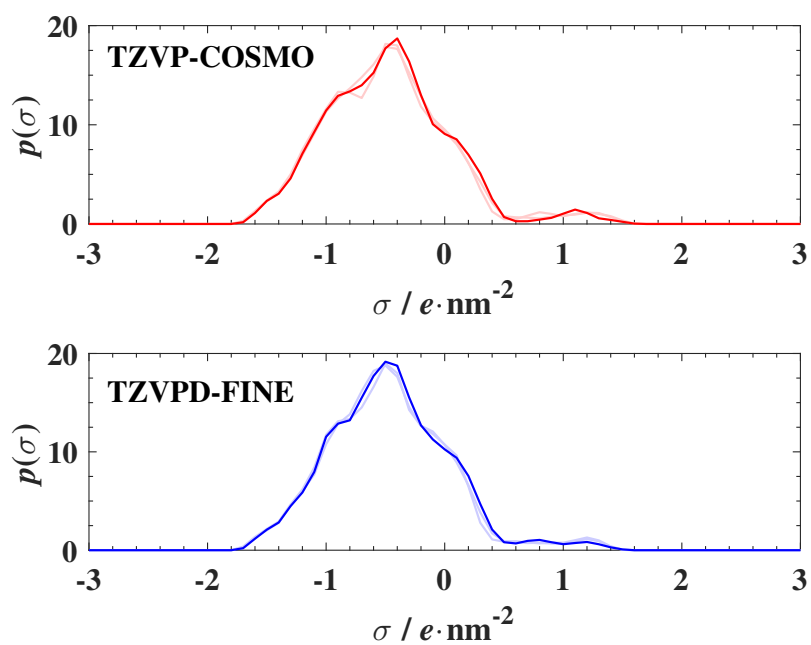




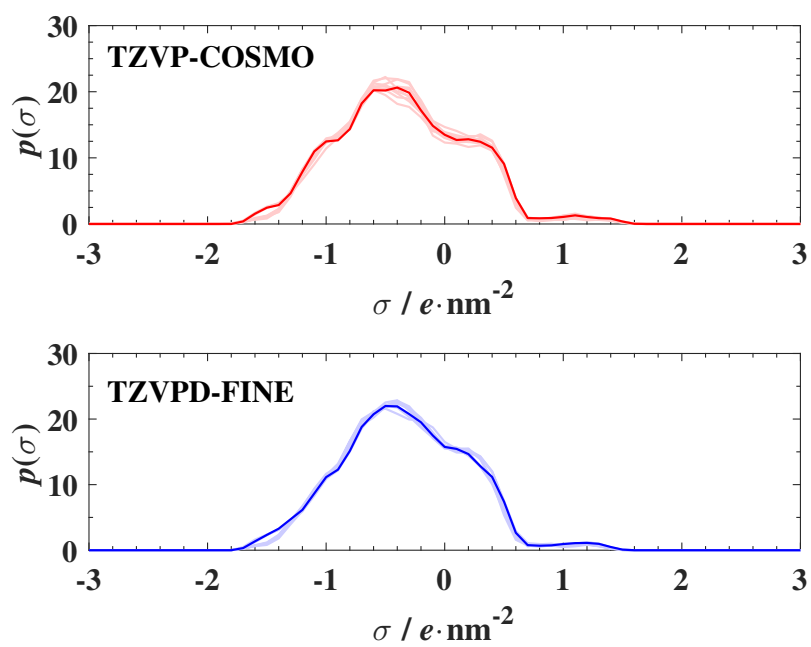
**Figure S21.**  $\sigma$ -profiles of IM-01,01 cation (abbreviations explained in the supplied Microsoft Excel spreadsheet, Table S1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



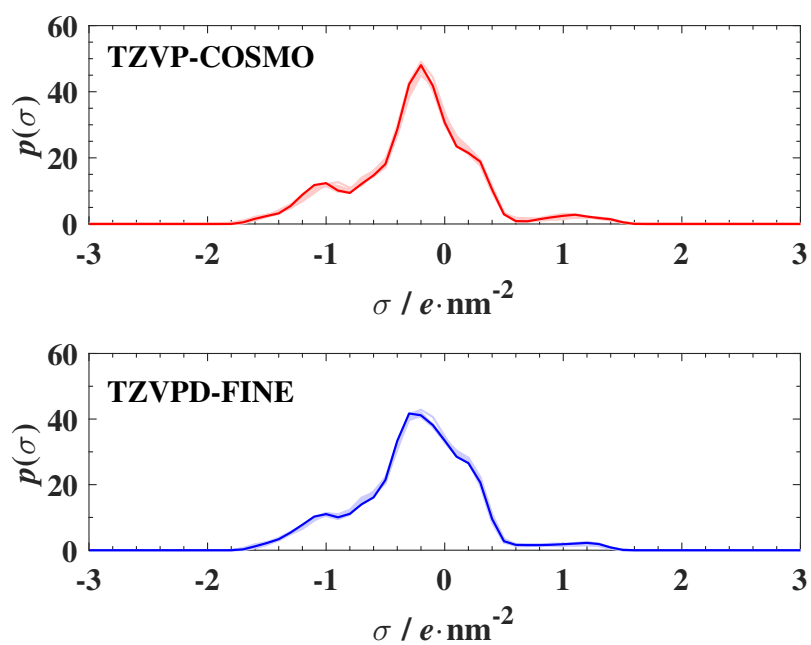
**Figure S22.**  $\sigma$ -profiles of IM-106, 1 cation (abbreviations explained in the supplied Microsoft Excel spreadsheet, Table S1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



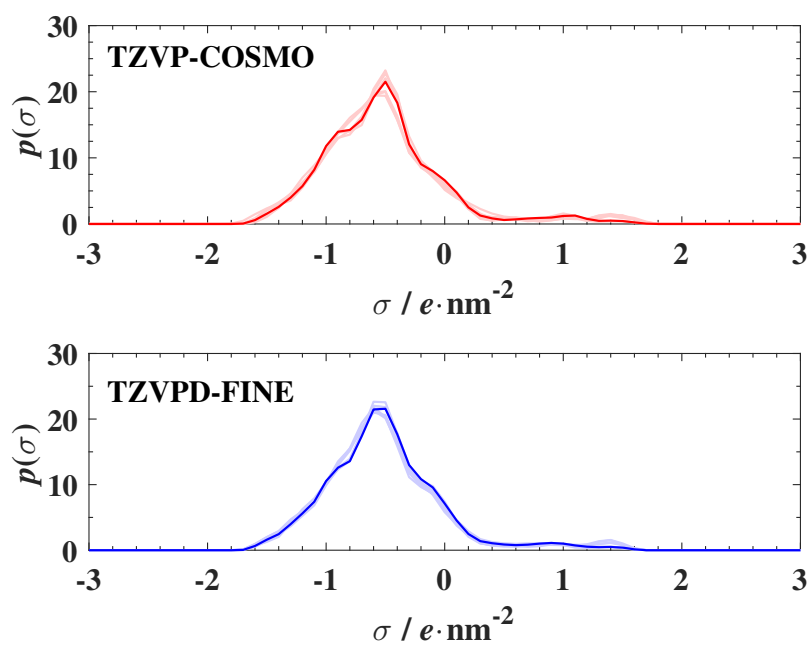
**Figure S23.**  $\sigma$ -profiles of IM-103, 1 cation (abbreviations explained in the supplied Microsoft Excel spreadsheet, Table S1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



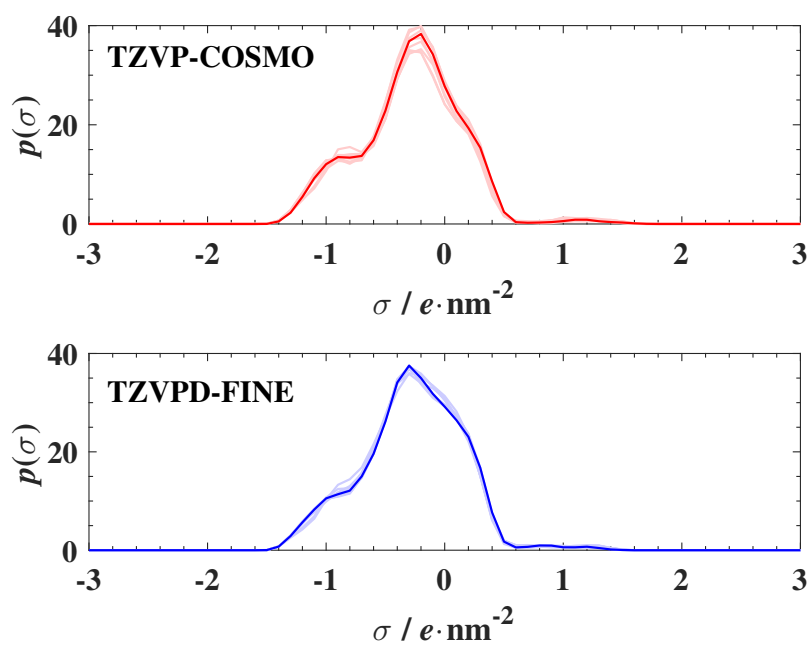
**Figure S24.**  $\sigma$ -profiles of IM-103, 1PH cation (abbreviations explained in the supplied Microsoft Excel spreadsheet, Table S1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



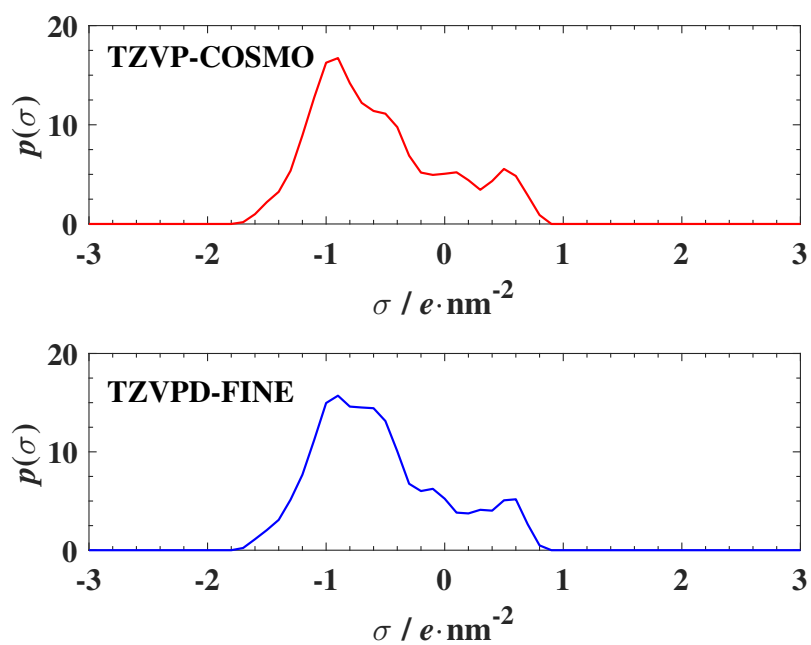
**Figure S25.**  $\sigma$ -profiles of IM-106, 106 cation (abbreviations explained in the supplied Microsoft Excel spreadsheet, Table S1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



**Figure S26.**  $\sigma$ -profiles of IM-201, 1 cation (abbreviations explained in the supplied Microsoft Excel spreadsheet, Table S1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).

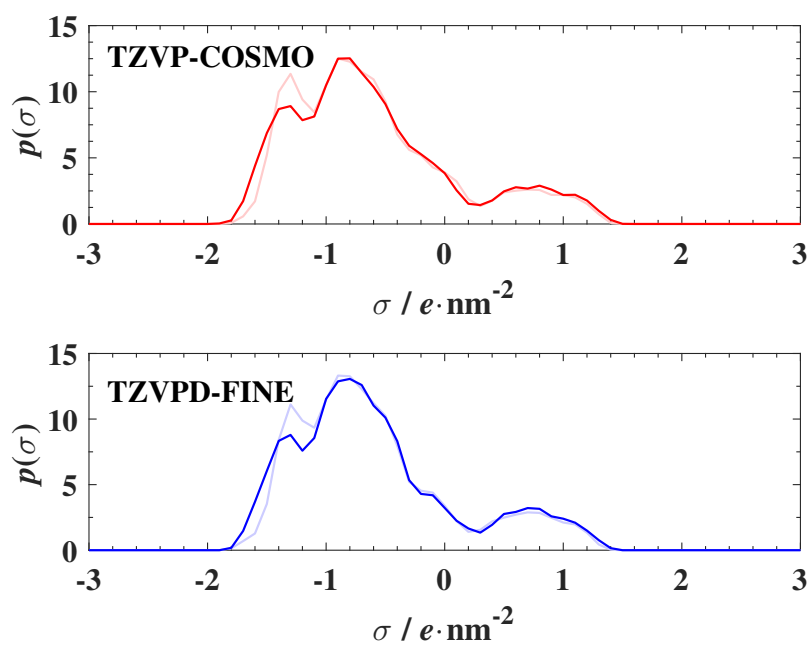


**Figure S27.**  $\sigma$ -profiles of IM-103, 8, 1 cation (abbreviations explained in the supplied Microsoft Excel spreadsheet, Table S1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).

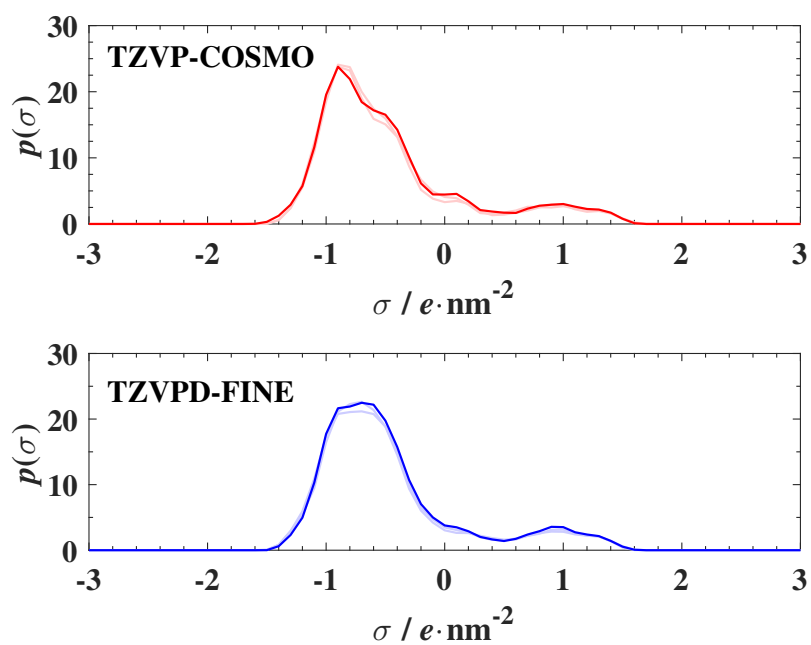


**Figure S28.**  $\sigma$ -profiles of IM-2CL, 1 cation (abbreviations explained in the supplied Microsoft Excel spreadsheet, Table S1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).

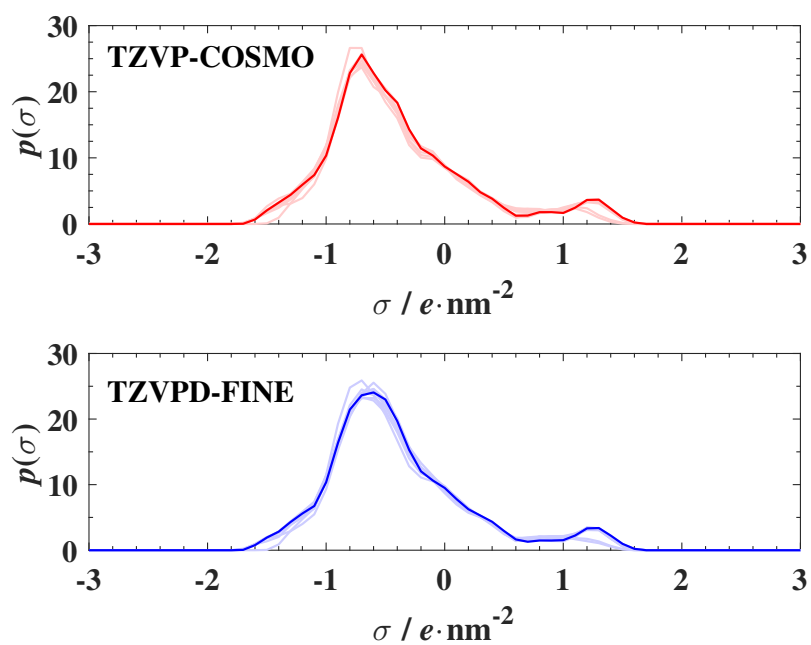




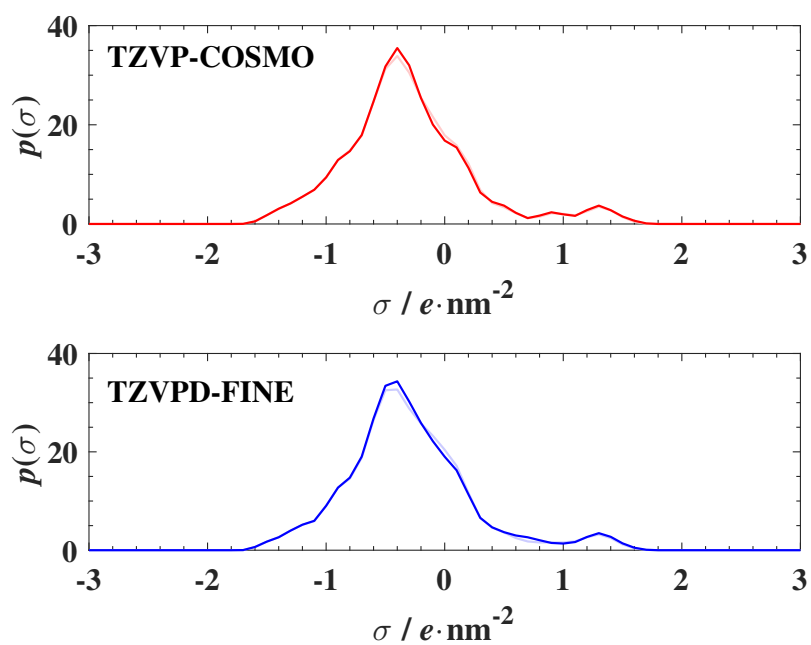
**Figure S29.**  $\sigma$ -profiles of IM-3CN, 1 cation (abbreviations explained in the supplied Microsoft Excel spreadsheet, Table S1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



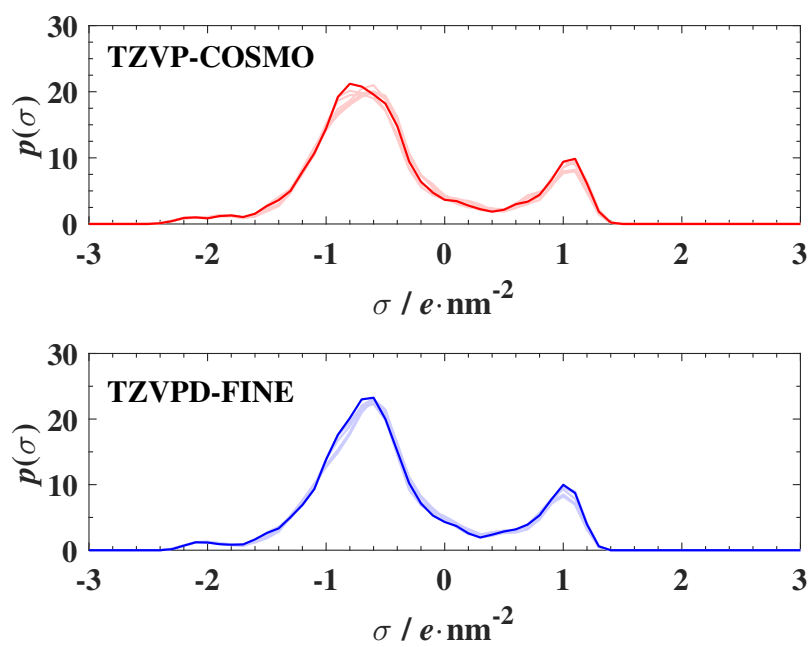
**Figure S30.**  $\sigma$ -profiles of IM-3CN, 1, 1 cation (abbreviations explained in the supplied Microsoft Excel spreadsheet, Table S1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



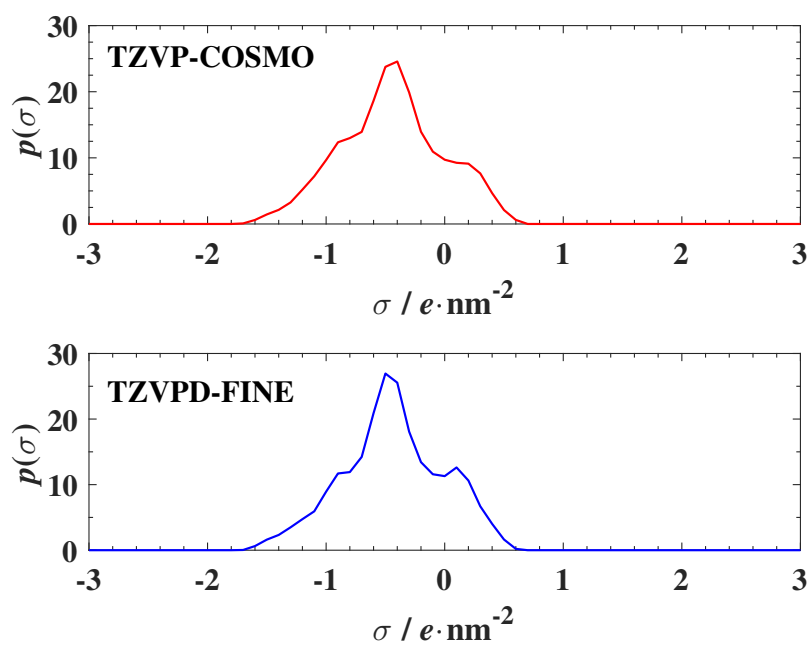
**Figure S31.**  $\sigma$ -profiles of IM-30ACRYLL, 1 cation (abbreviations explained in the supplied Microsoft Excel spreadsheet, Table S1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



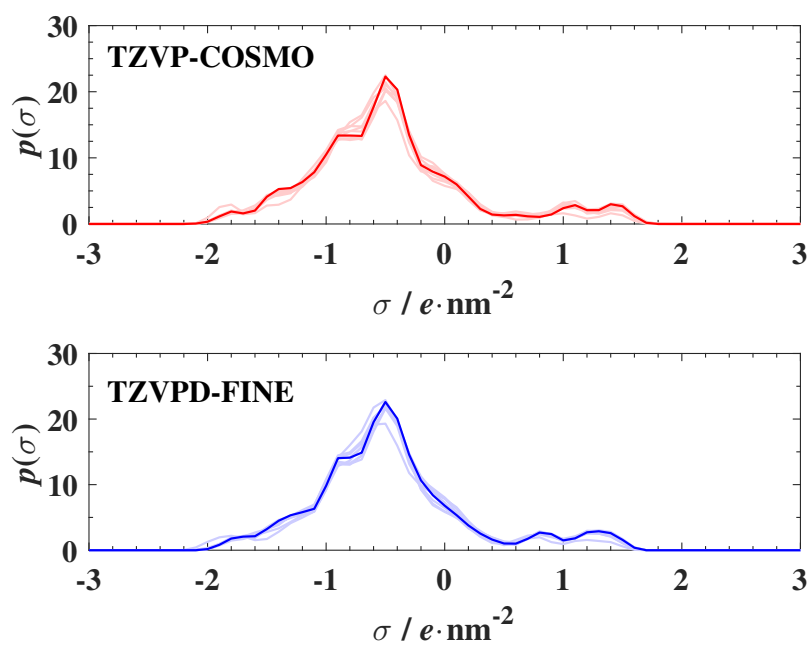
**Figure S32.**  $\sigma$ -profiles of IM-60ACRYLL, 1 cation (abbreviations explained in the supplied Microsoft Excel spreadsheet, Table S1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



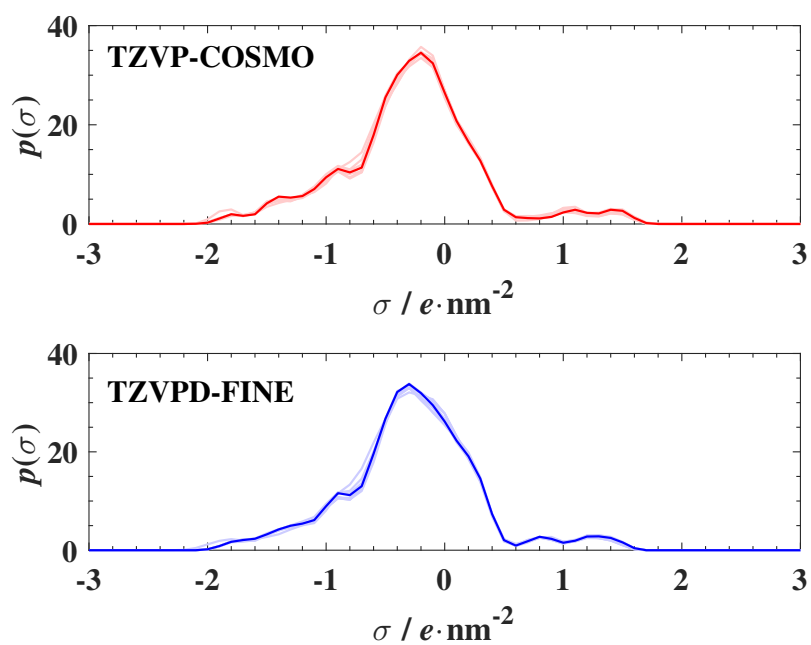
**Figure S33.**  $\sigma$ -profiles of IM-4SO3H, 1 cation (abbreviations explained in the supplied Microsoft Excel spreadsheet, Table S1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



**Figure S34.**  $\sigma$ -profiles of IM-1TMS, 1 cation (abbreviations explained in the supplied Microsoft Excel spreadsheet, Table S1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).

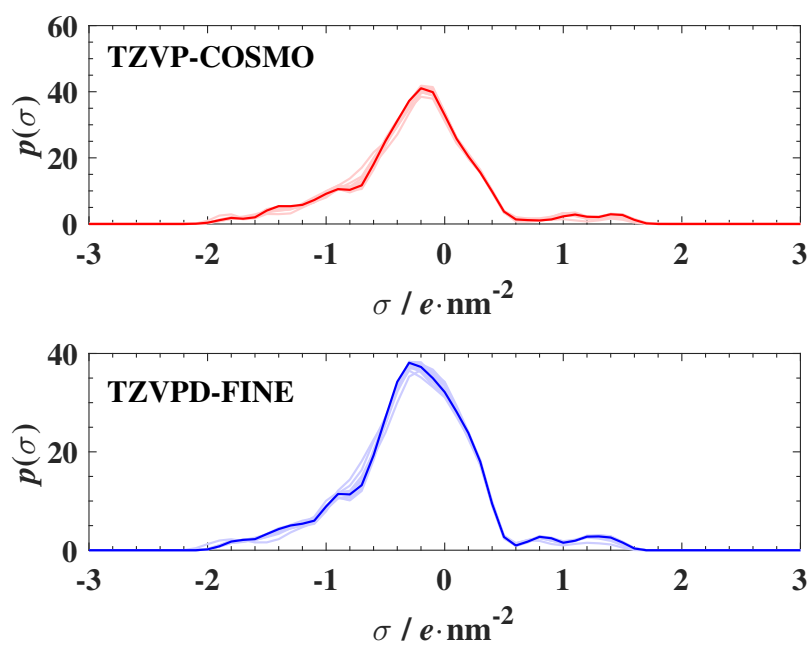


**Figure S35.**  $\sigma$ -profiles of IM-3B(OH)<sub>2</sub>, 1 cation (abbreviations explained in the supplied Microsoft Excel spreadsheet, Table S1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).

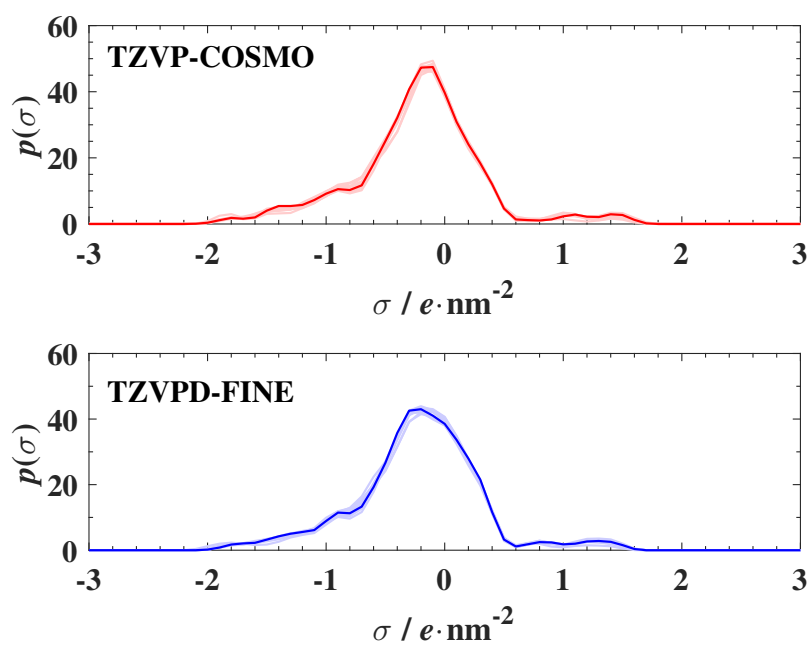


**Figure S36.**  $\sigma$ -profiles of IM-3B(OH)<sub>2</sub>, 8 cation (abbreviations explained in the supplied Microsoft Excel spreadsheet, Table S1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).

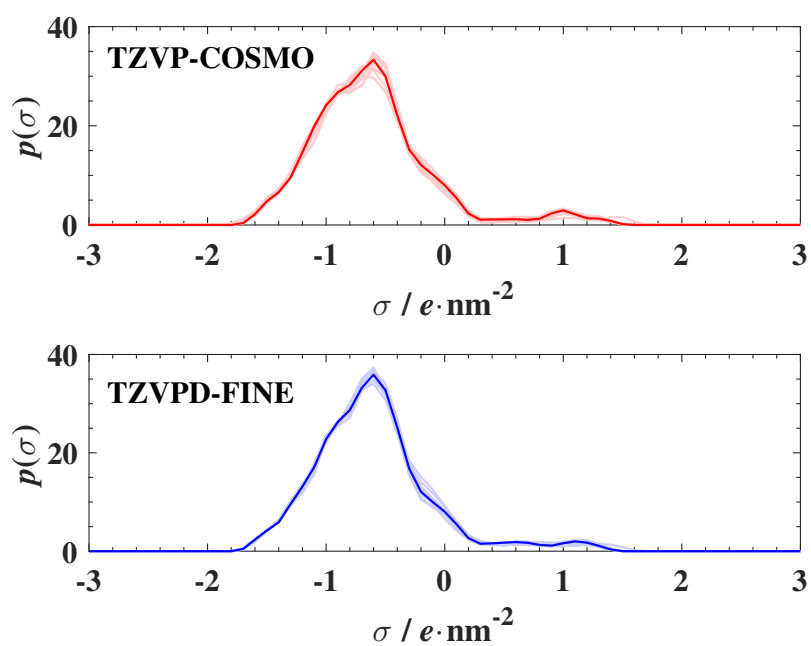




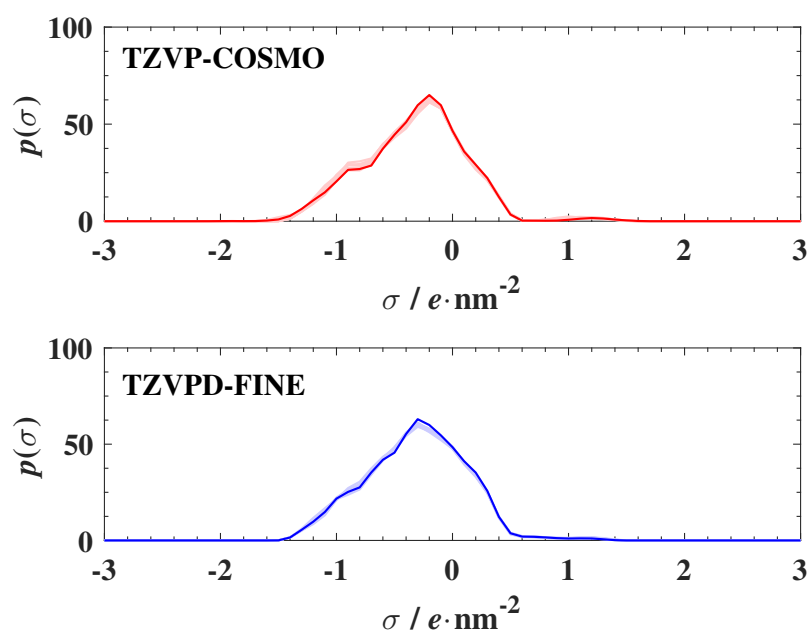
**Figure S37.**  $\sigma$ -profiles of IM-3B(OH)<sub>2</sub>, 10 cation (abbreviations explained in the supplied Microsoft Excel spreadsheet, Table S1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



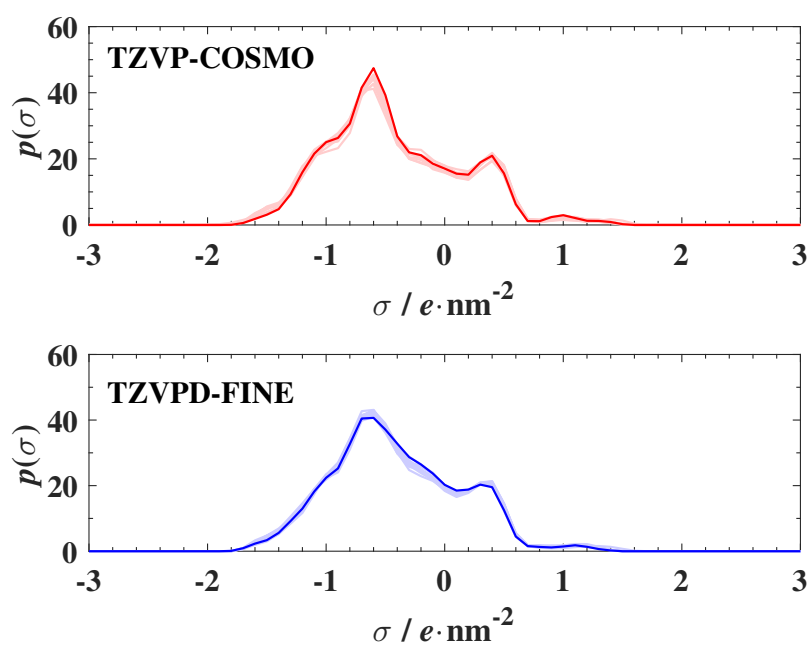
**Figure S38.**  $\sigma$ -profiles of IM-3B(OH)<sub>2</sub>,<sub>12</sub> cation (abbreviations explained in the supplied Microsoft Excel spreadsheet, Table S1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



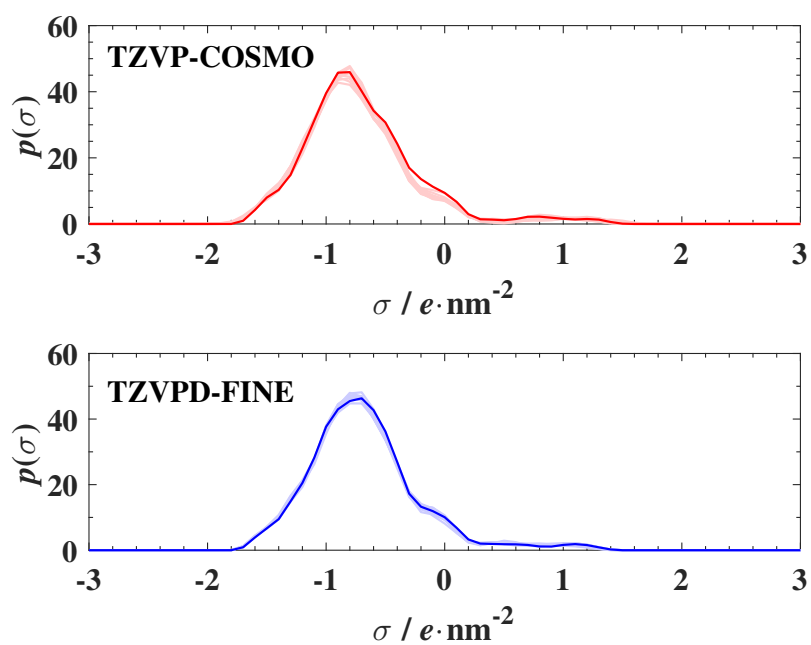
**Figure S39.**  $\sigma$ -profiles of DC[IM-1]2-10301 cation (abbreviations explained in the supplied Microsoft Excel spreadsheet, Table S1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



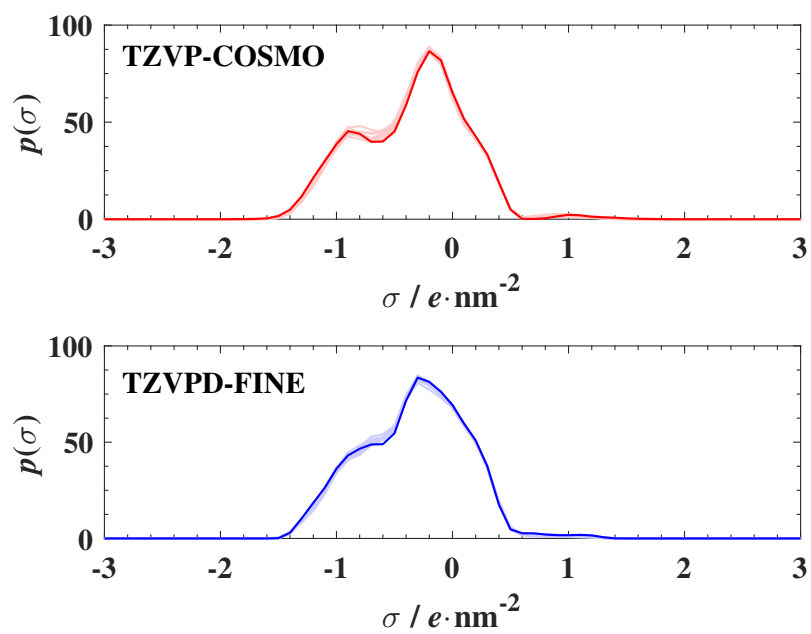
**Figure S40.**  $\sigma$ -profiles of DC[IM-8, 1]2-10301 cation (abbreviations explained in the supplied Microsoft Excel spreadsheet, Table S1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



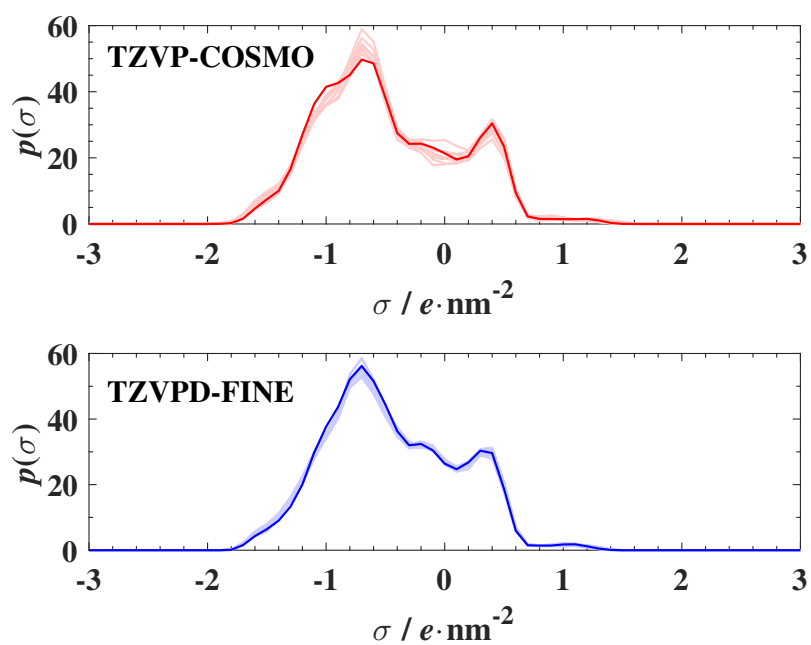
**Figure S41.**  $\sigma$ -profiles of DC[IM-1PH]2-10301 cation (abbreviations explained in the supplied Microsoft Excel spreadsheet, Table S1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



**Figure S42.**  $\sigma$ -profiles of TC[MUTELET1A] cation (abbreviations explained in the supplied Microsoft Excel spreadsheet, Table S1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).

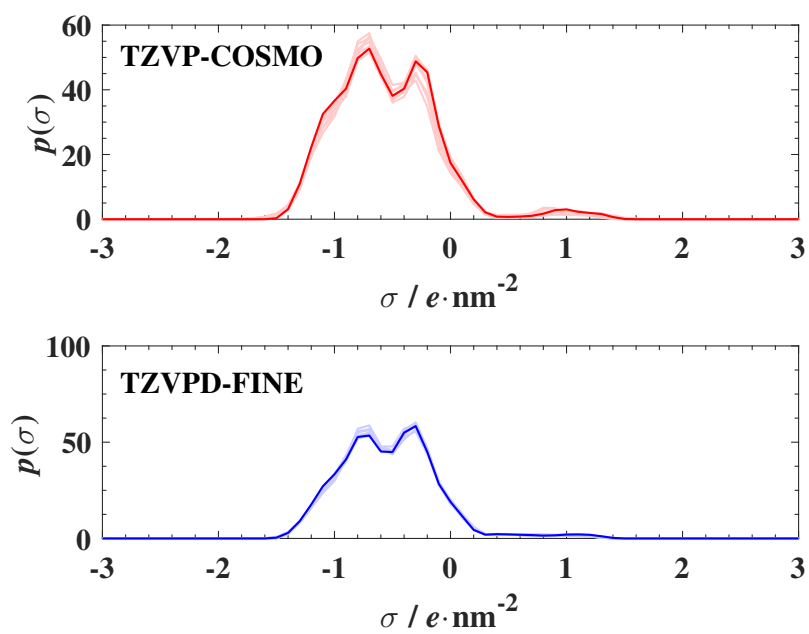


**Figure S43.**  $\sigma$ -profiles of TC[MUTELET1C] cation (abbreviations explained in the supplied Microsoft Excel spreadsheet, Table S1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).

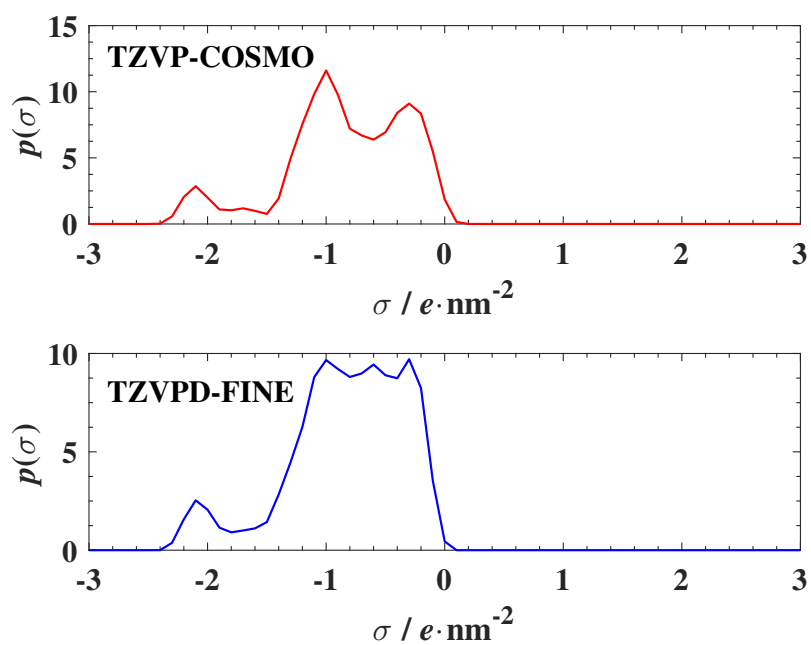


**Figure S44.**  $\sigma$ -profiles of TC[MUTELET1E] cation (abbreviations explained in the supplied Microsoft Excel spreadsheet, Table S1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).

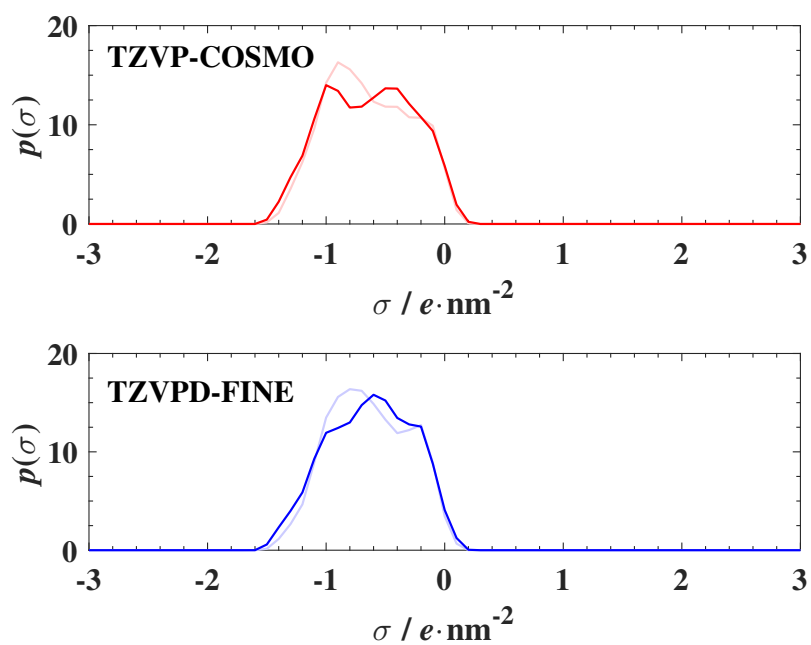




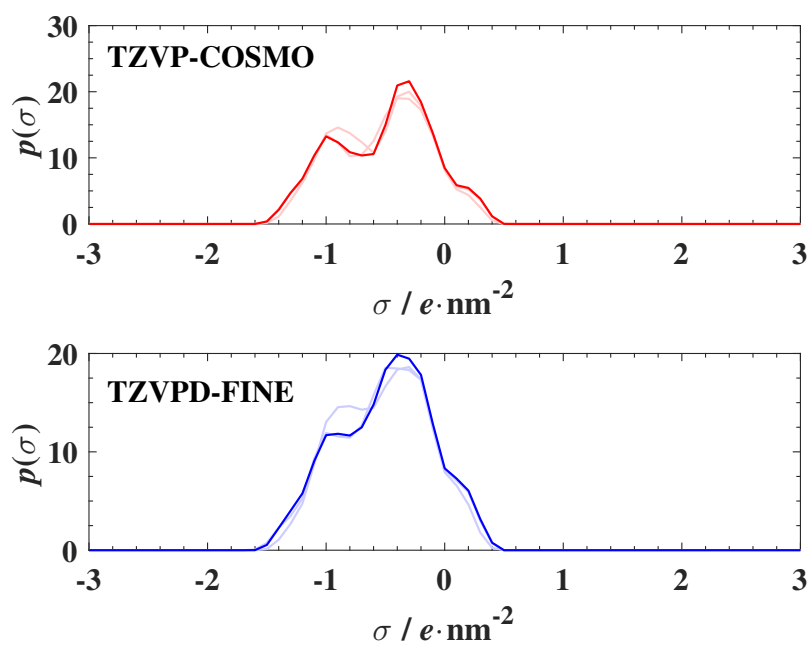
**Figure S45.**  $\sigma$ -profiles of TC[MUTELET2A] cation (abbreviations explained in the supplied Microsoft Excel spreadsheet, Table S1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



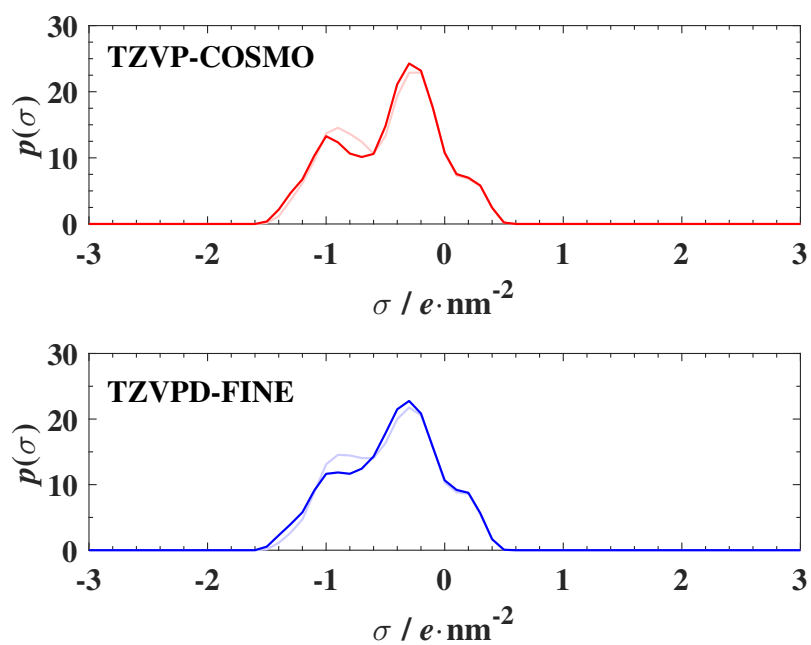
**Figure S46.**  $\sigma$ -profiles of PY cation (abbreviations explained in the supplied Microsoft Excel spreadsheet, Table S1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



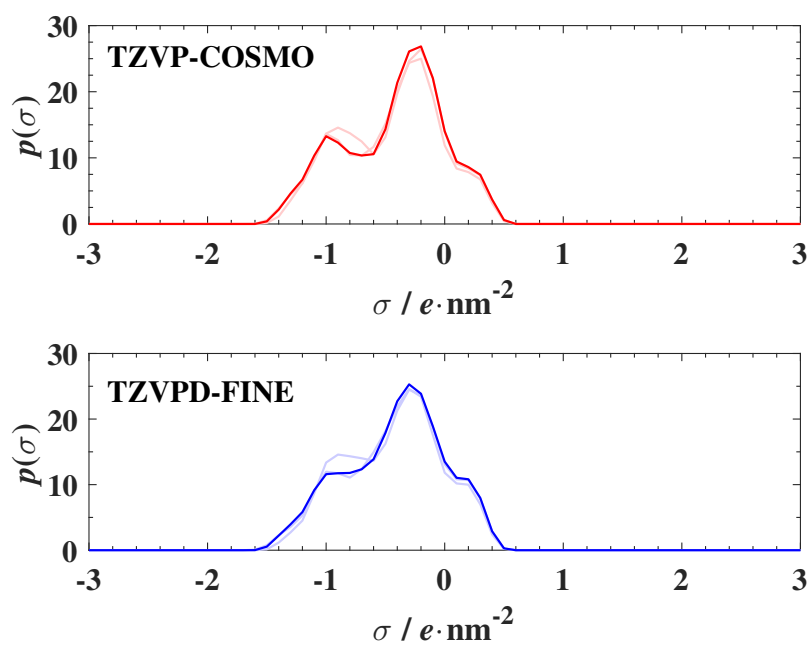
**Figure S47.**  $\sigma$ -profiles of PY-2 cation (abbreviations explained in the supplied Microsoft Excel spreadsheet, Table S1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



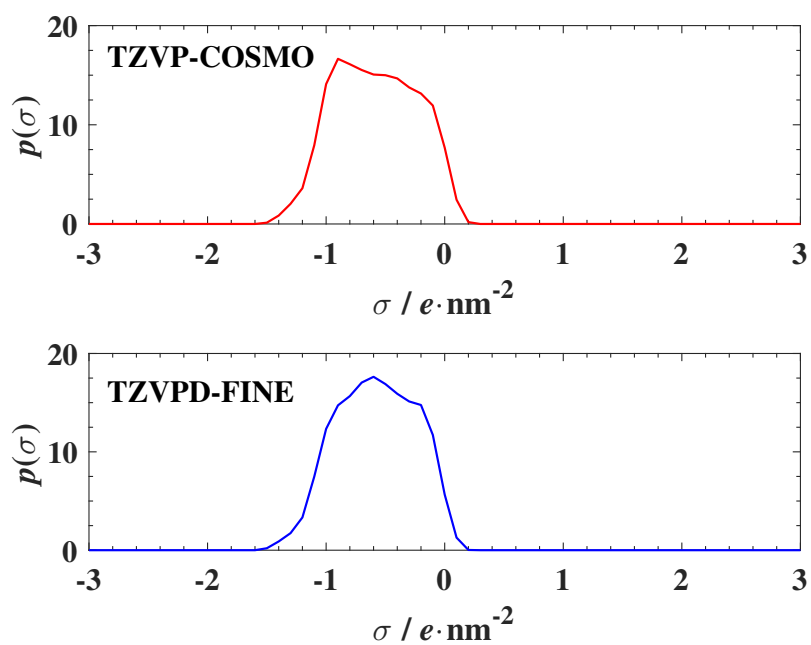
**Figure S48.**  $\sigma$ -profiles of PY-4 cation (abbreviations explained in the supplied Microsoft Excel spreadsheet, Table S1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



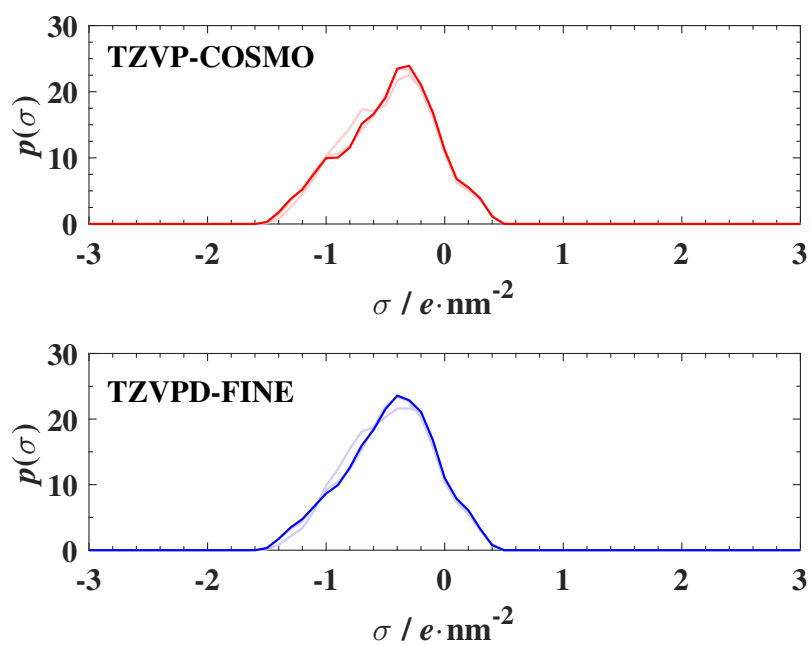
**Figure S49.**  $\sigma$ -profiles of PY-5 cation (abbreviations explained in the supplied Microsoft Excel spreadsheet, Table S1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



**Figure S50.**  $\sigma$ -profiles of PY-6 cation (abbreviations explained in the supplied Microsoft Excel spreadsheet, Table S1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).

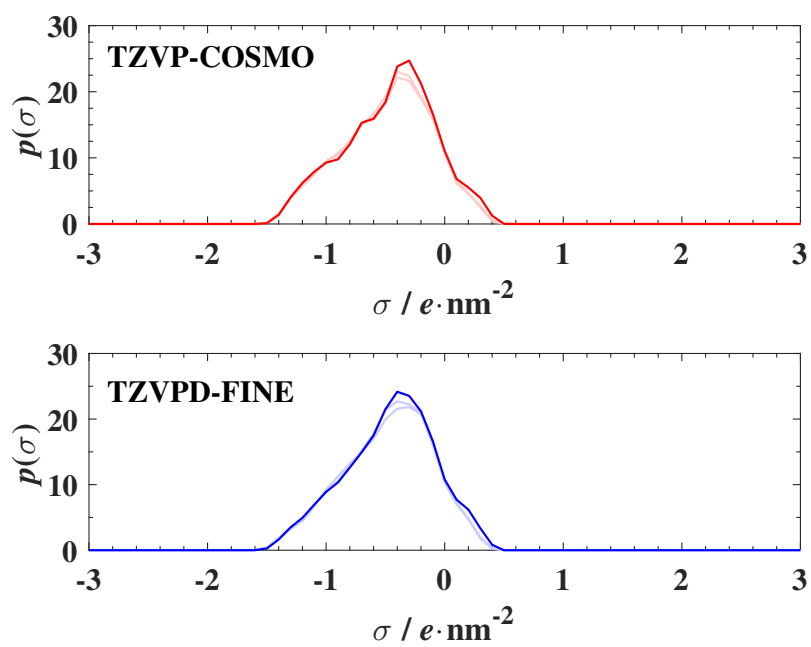


**Figure S51.**  $\sigma$ -profiles of PY-2, 1[2] cation (abbreviations explained in the supplied Microsoft Excel spreadsheet, Table S1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).

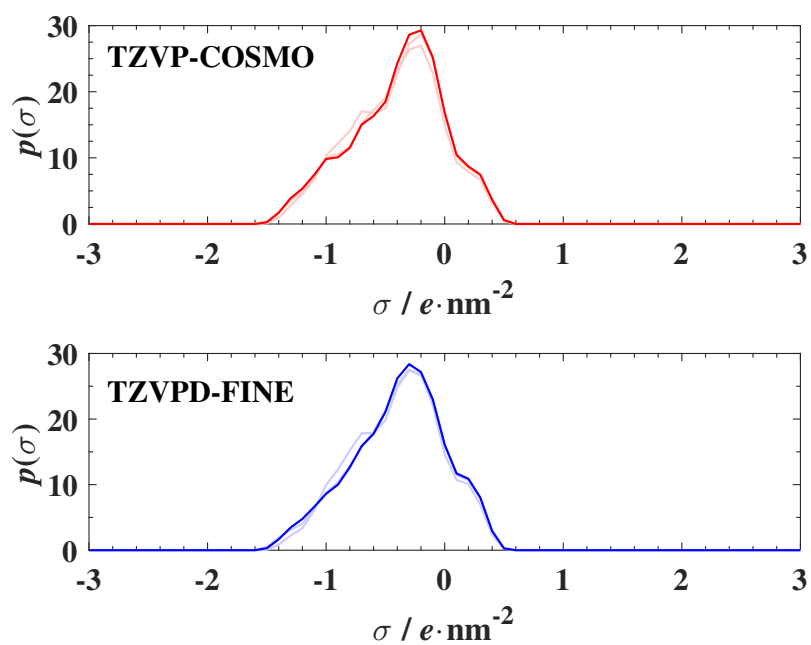


**Figure S52.**  $\sigma$ -profiles of PY-4, 1[3] cation (abbreviations explained in the supplied Microsoft Excel spreadsheet, Table S1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).

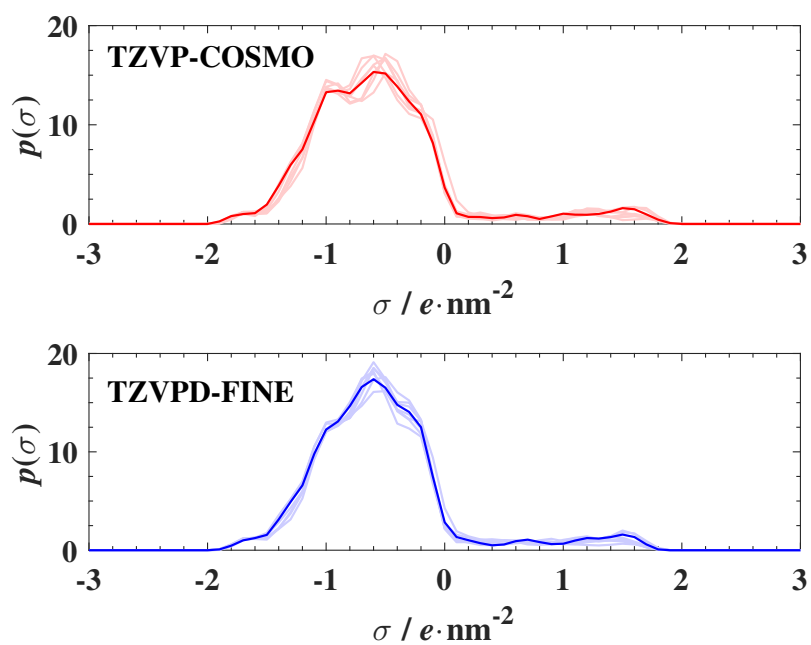




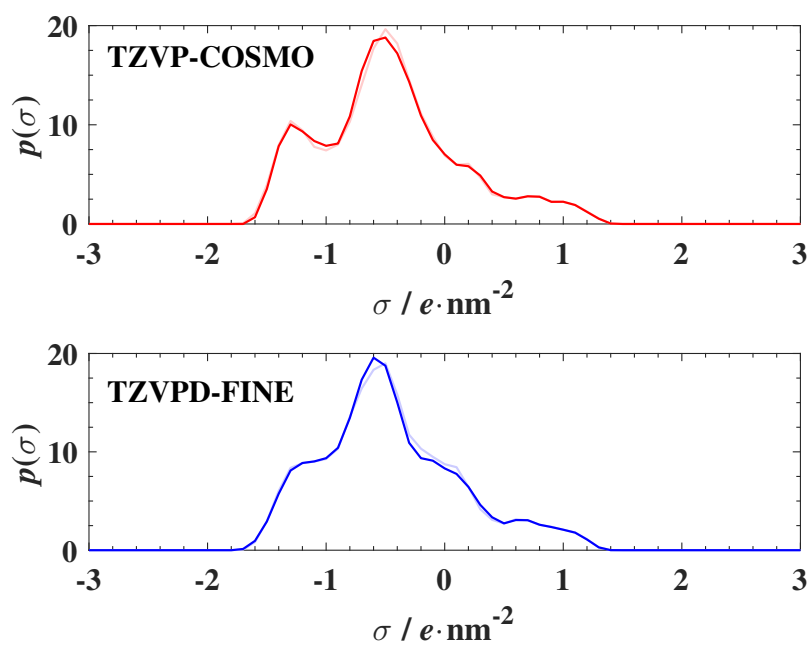
**Figure S53.**  $\sigma$ -profiles of PY-4, 1[4] cation (abbreviations explained in the supplied Microsoft Excel spreadsheet, Table S1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



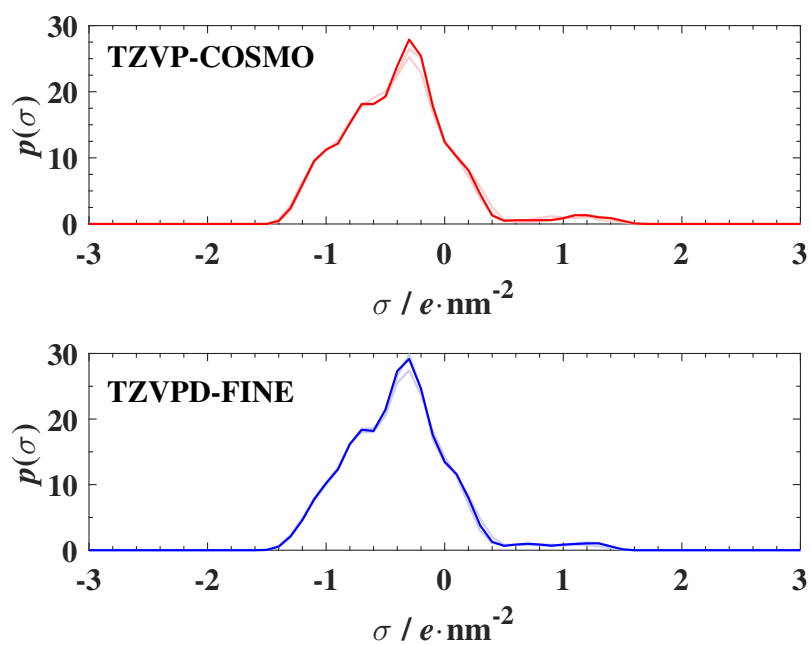
**Figure S54.**  $\sigma$ -profiles of PY-6, 1[3] cation (abbreviations explained in the supplied Microsoft Excel spreadsheet, Table S1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



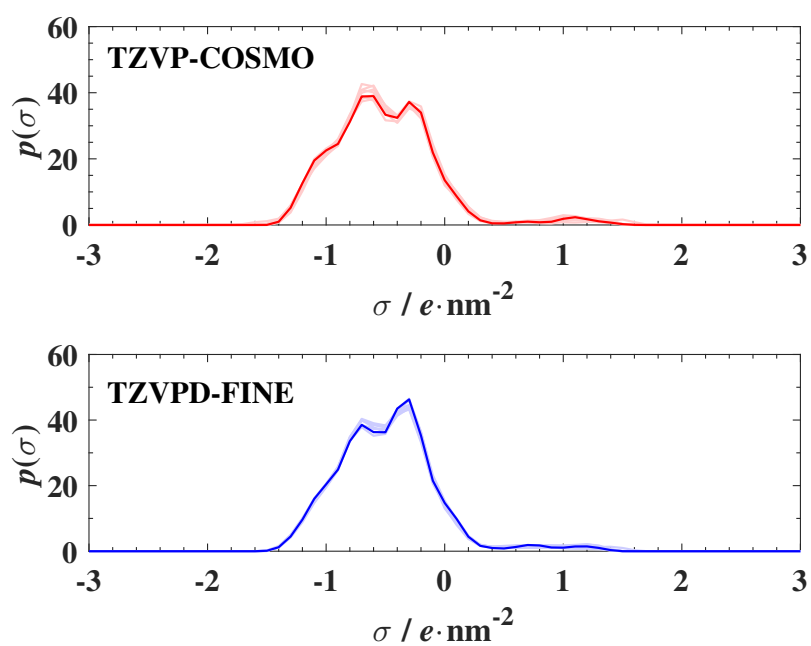
**Figure S55.**  $\sigma$ -profiles of PY-30H cation (abbreviations explained in the supplied Microsoft Excel spreadsheet, Table S1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



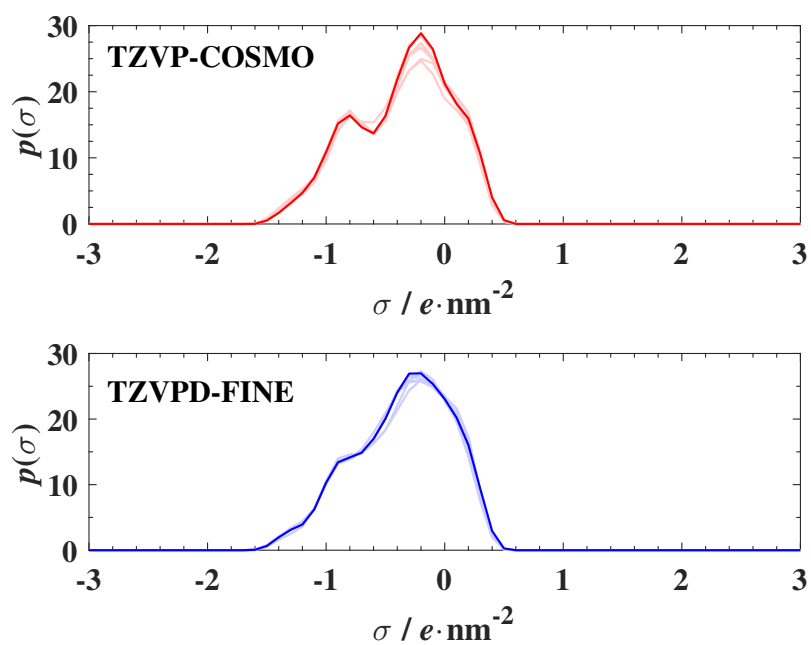
**Figure S56.**  $\sigma$ -profiles of PY-4, CN[4] cation (abbreviations explained in the supplied Microsoft Excel spreadsheet, Table S1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



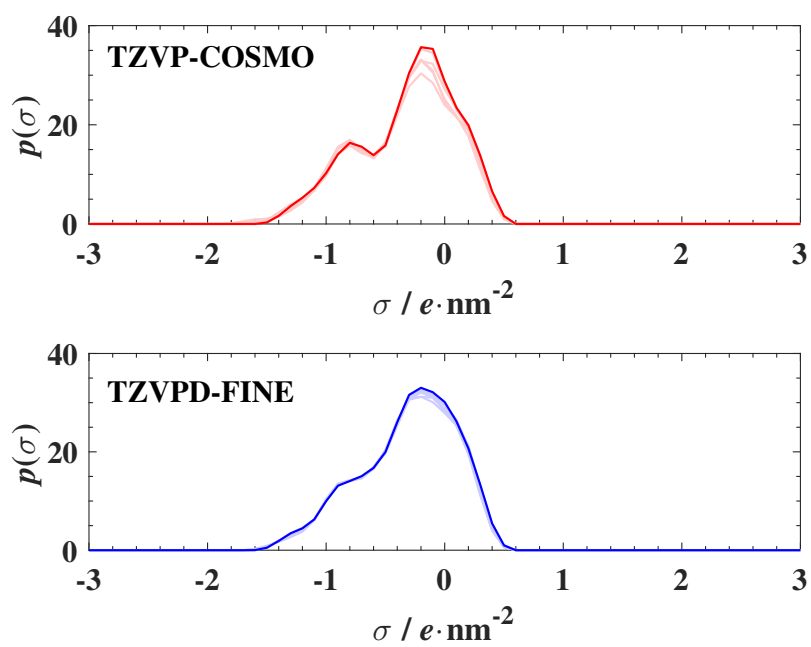
**Figure S57.**  $\sigma$ -profiles of PY-103, DMA[4] cation (abbreviations explained in the supplied Microsoft Excel spreadsheet, Table S1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



**Figure S58.**  $\sigma$ -profiles of DC[PY-DMA[4]]<sub>2</sub>-10301 cation (abbreviations explained in the supplied Microsoft Excel spreadsheet, Table S1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).

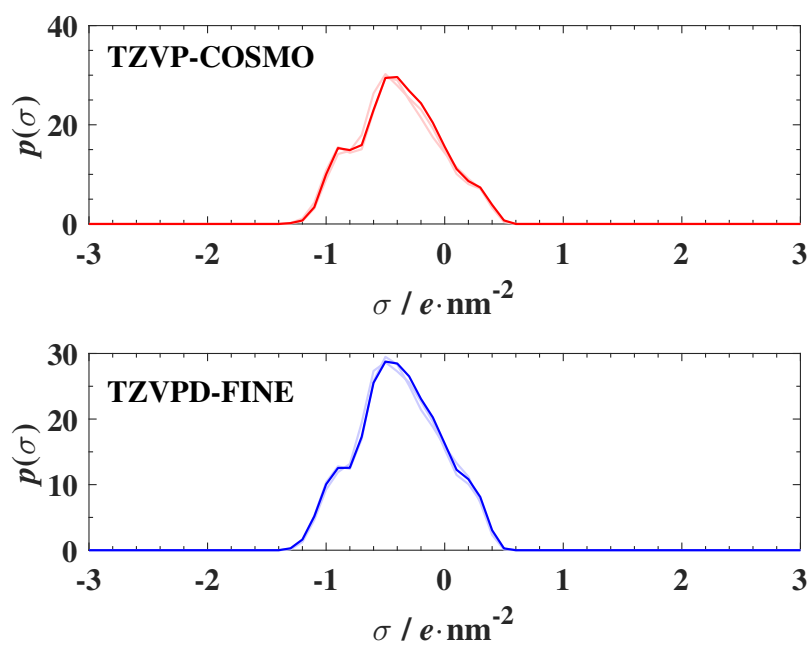


**Figure S59.**  $\sigma$ -profiles of QUINI-6 cation (abbreviations explained in the supplied Microsoft Excel spreadsheet, Table S1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).

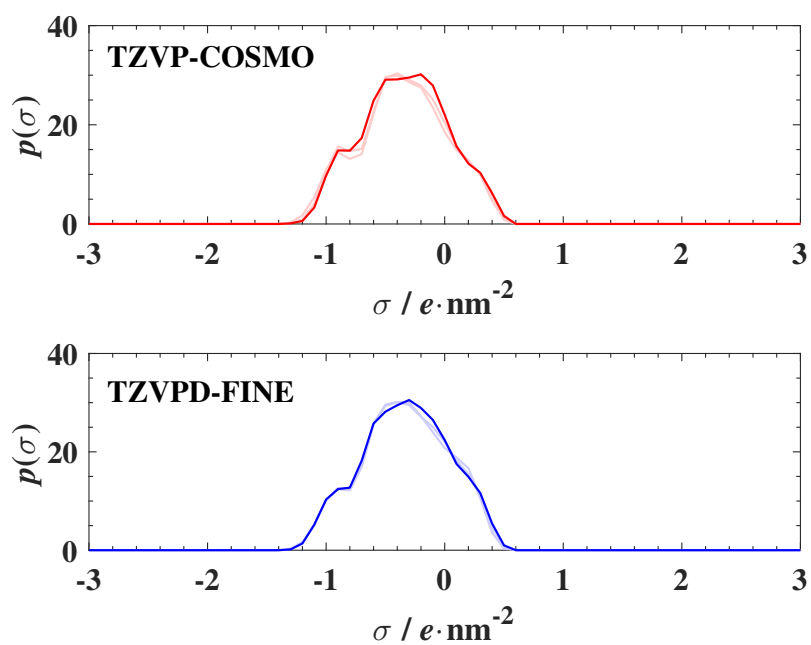


**Figure S60.**  $\sigma$ -profiles of QUINI-8 cation (abbreviations explained in the supplied Microsoft Excel spreadsheet, Table S1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).

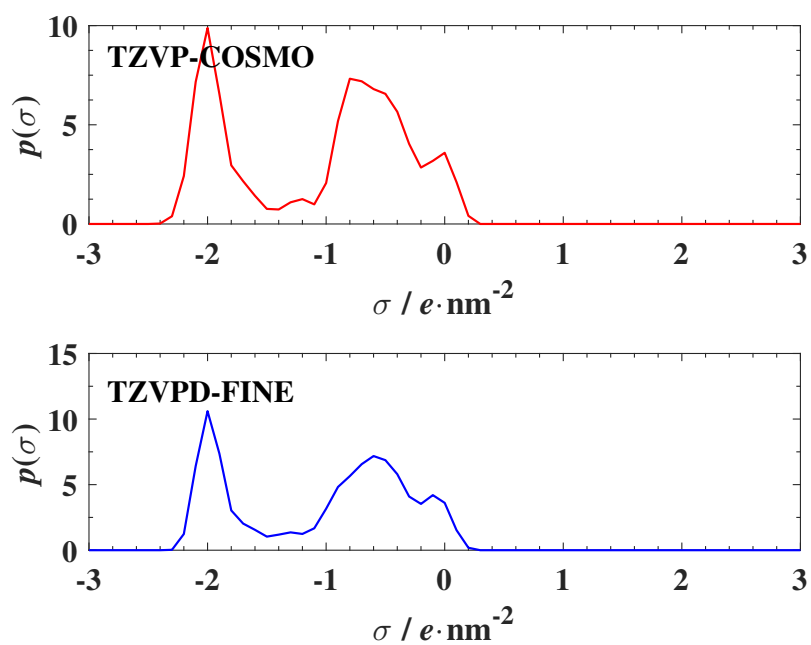




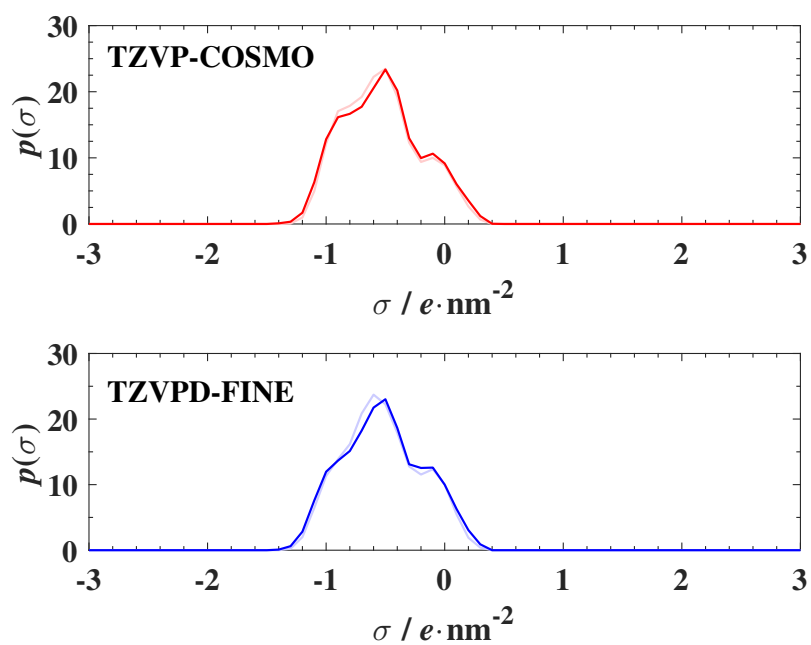
**Figure S61.**  $\sigma$ -profiles of QUINUC-6 cation (abbreviations explained in the supplied Microsoft Excel spreadsheet, Table S1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



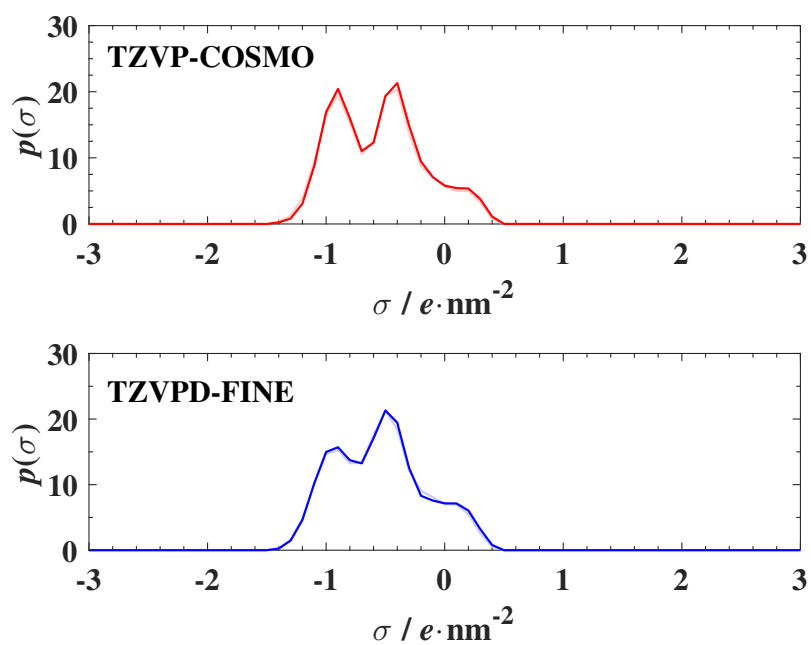
**Figure S62.**  $\sigma$ -profiles of QUINUC-8 cation (abbreviations explained in the supplied Microsoft Excel spreadsheet, Table S1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



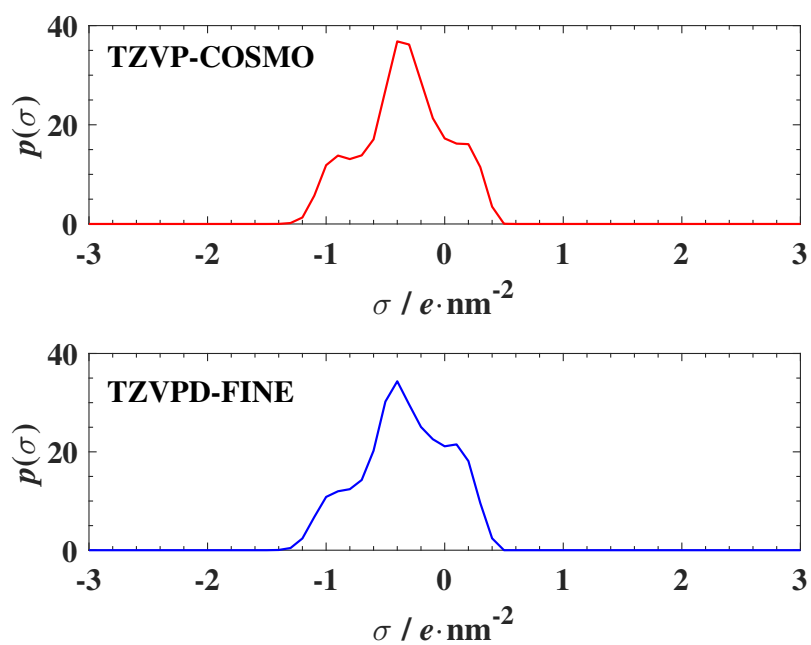
**Figure S63.**  $\sigma$ -profiles of N-2 cation (abbreviations explained in the supplied Microsoft Excel spreadsheet, Table S1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



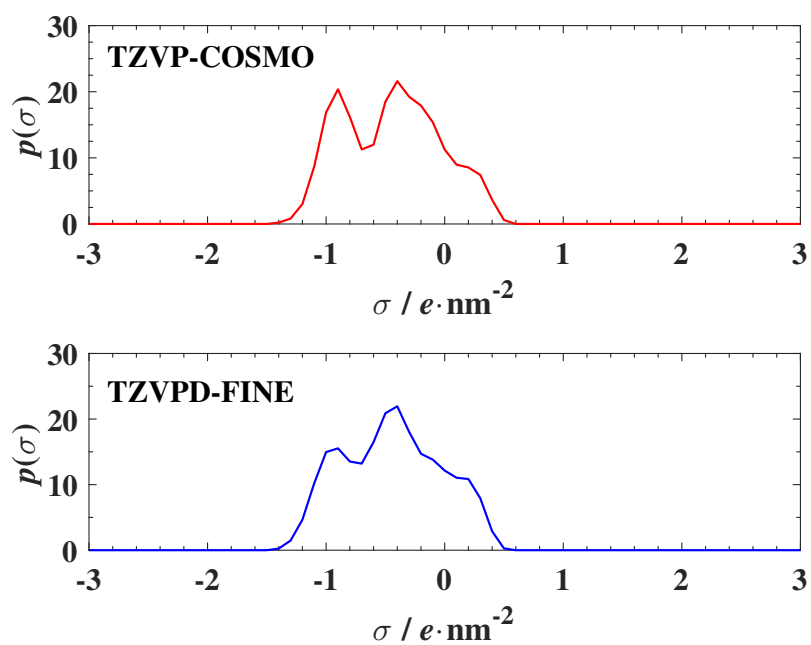
**Figure S64.**  $\sigma$ -profiles of N-3, 3I, 1, 1 cation (abbreviations explained in the supplied Microsoft Excel spreadsheet, Table S1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



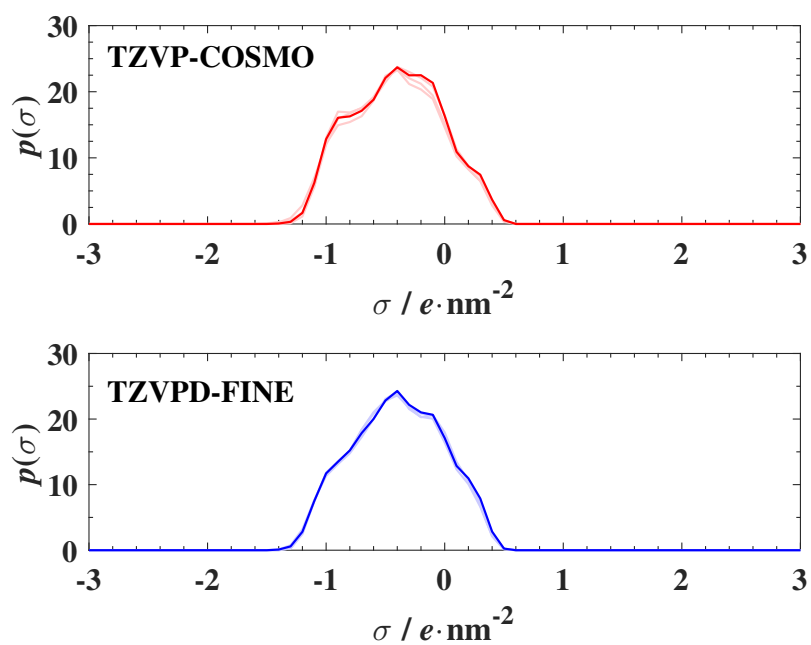
**Figure S65.**  $\sigma$ -profiles of N-4, 1, 1, 1 cation (abbreviations explained in the supplied Microsoft Excel spreadsheet, Table S1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



**Figure S66.**  $\sigma$ -profiles of N-4, 4, 4, 1 cation (abbreviations explained in the supplied Microsoft Excel spreadsheet, Table S1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).

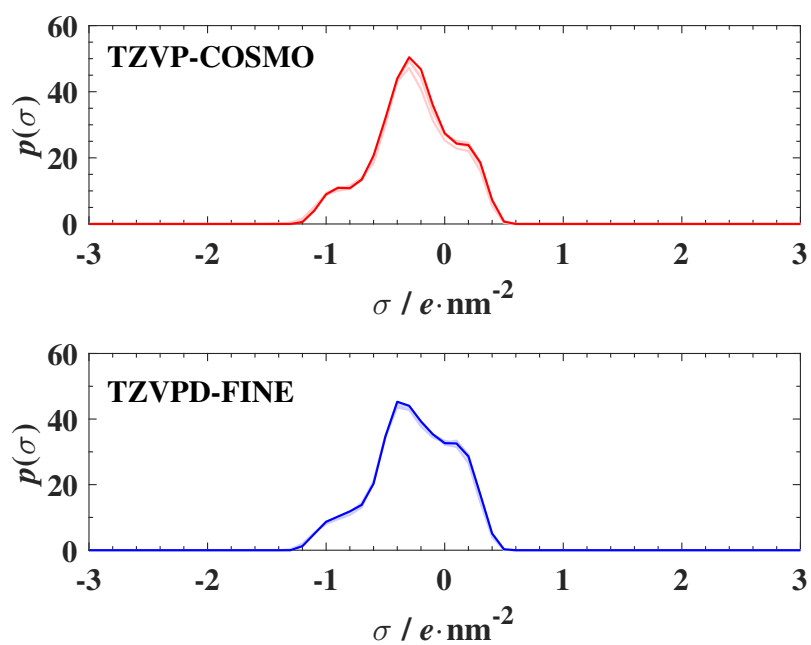


**Figure S67.**  $\sigma$ -profiles of N-6, 1, 1, 1 cation (abbreviations explained in the supplied Microsoft Excel spreadsheet, Table S1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).

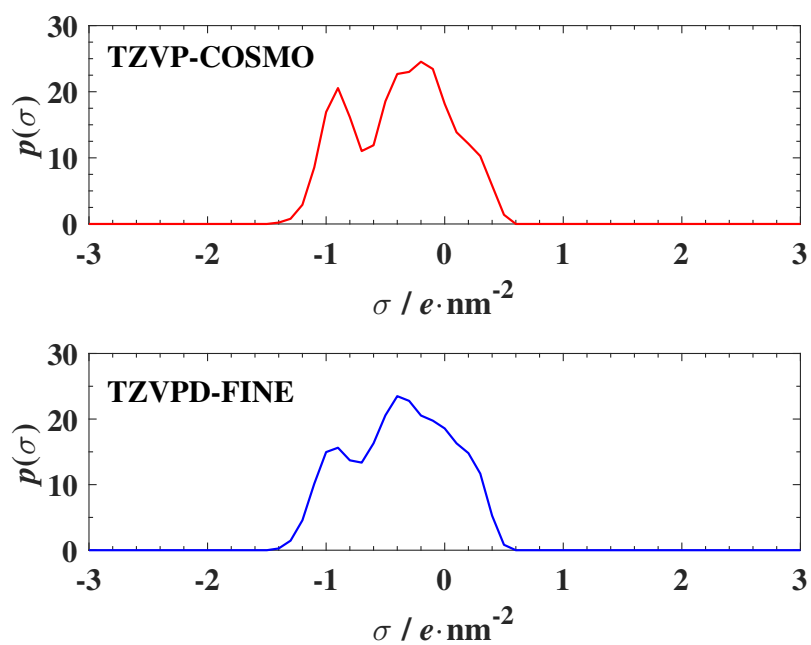


**Figure S68.**  $\sigma$ -profiles of N-6, 3I, 1, 1 cation (abbreviations explained in the supplied Microsoft Excel spreadsheet, Table S1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).

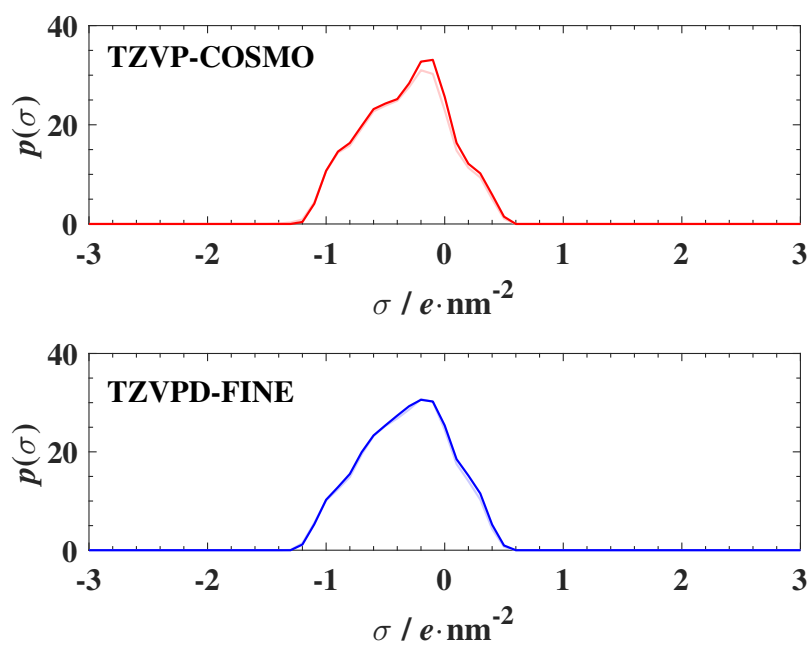




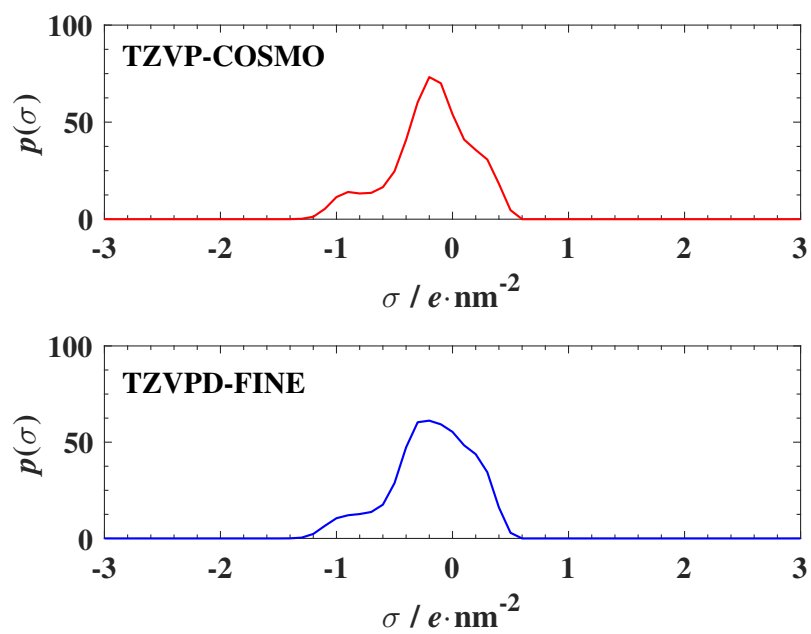
**Figure S69.**  $\sigma$ -profiles of N-6, 4, 4, 4 cation (abbreviations explained in the supplied Microsoft Excel spreadsheet, Table S1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



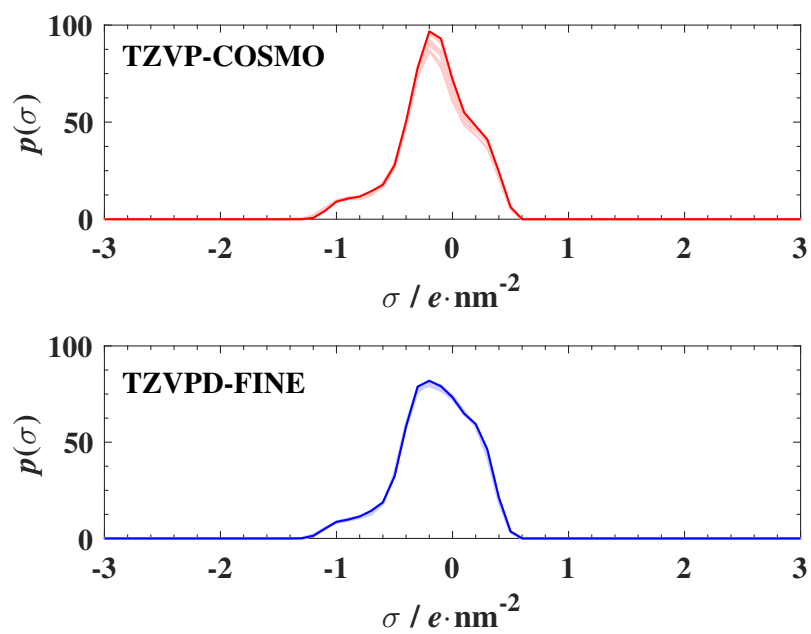
**Figure S70.**  $\sigma$ -profiles of N-8, 1, 1, 1 cation (abbreviations explained in the supplied Microsoft Excel spreadsheet, Table S1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



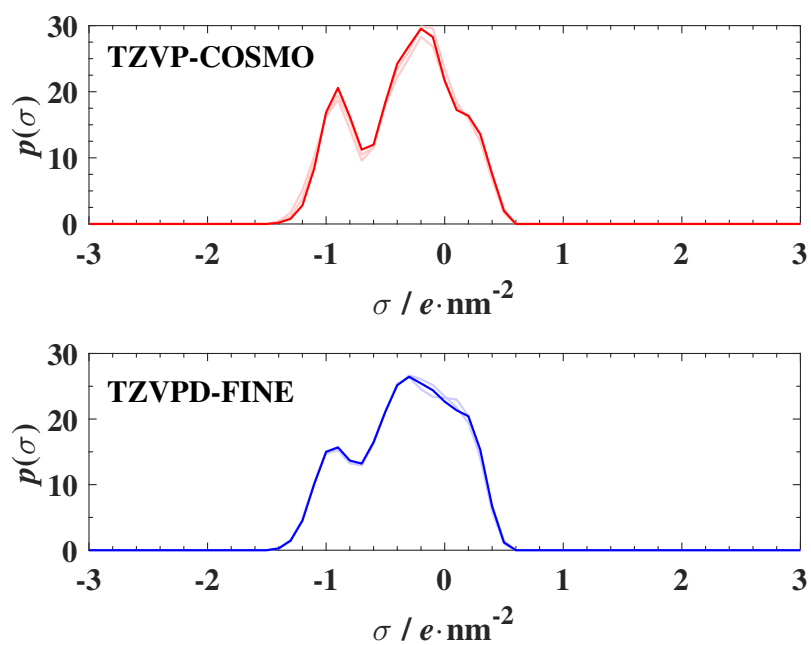
**Figure S71.**  $\sigma$ -profiles of N-8, 2, 2, 2 cation (abbreviations explained in the supplied Microsoft Excel spreadsheet, Table S1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



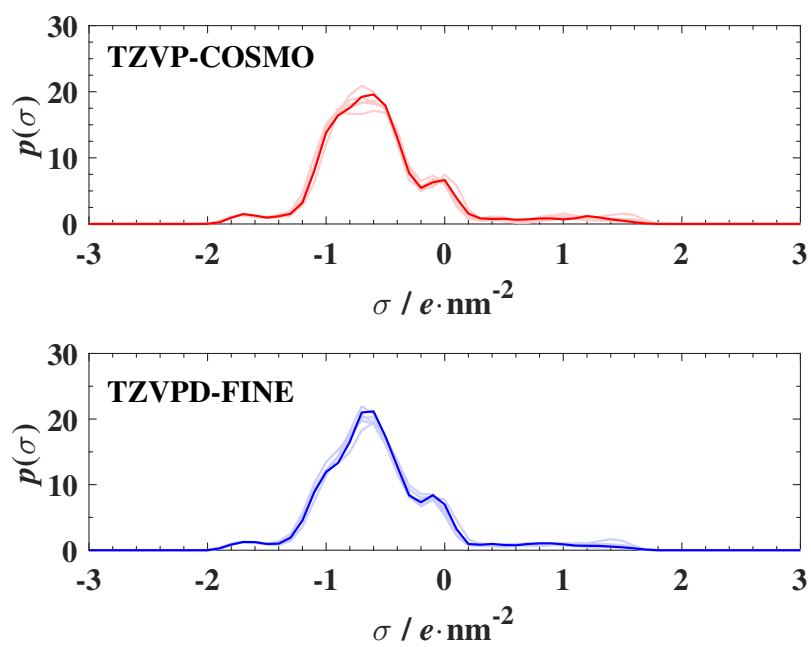
**Figure S72.**  $\sigma$ -profiles of N-8, 8, 8, 1 cation (abbreviations explained in the supplied Microsoft Excel spreadsheet, Table S1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



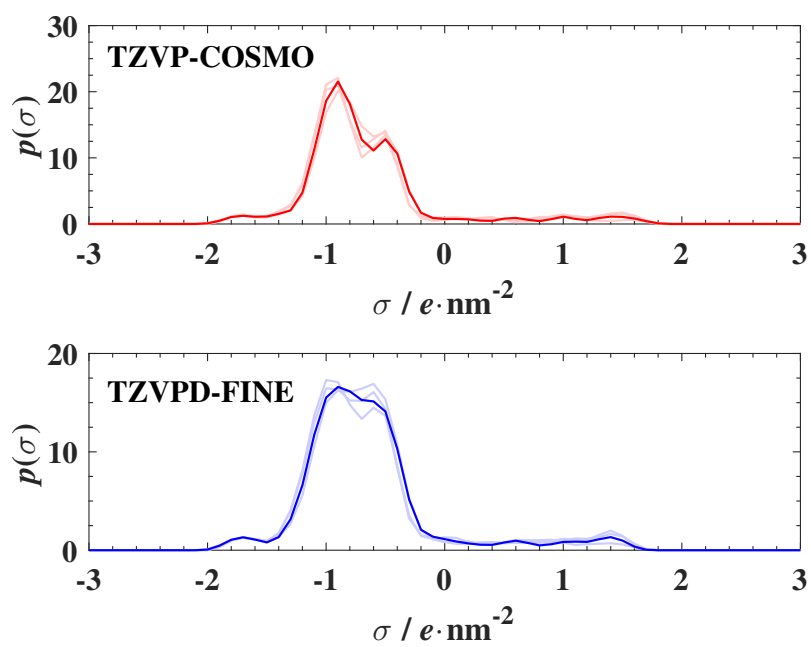
**Figure S73.**  $\sigma$ -profiles of N-8, 8, 8, 8 cation (abbreviations explained in the supplied Microsoft Excel spreadsheet, Table S1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



**Figure S74.**  $\sigma$ -profiles of N-10, 1, 1, 1 cation (abbreviations explained in the supplied Microsoft Excel spreadsheet, Table S1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).

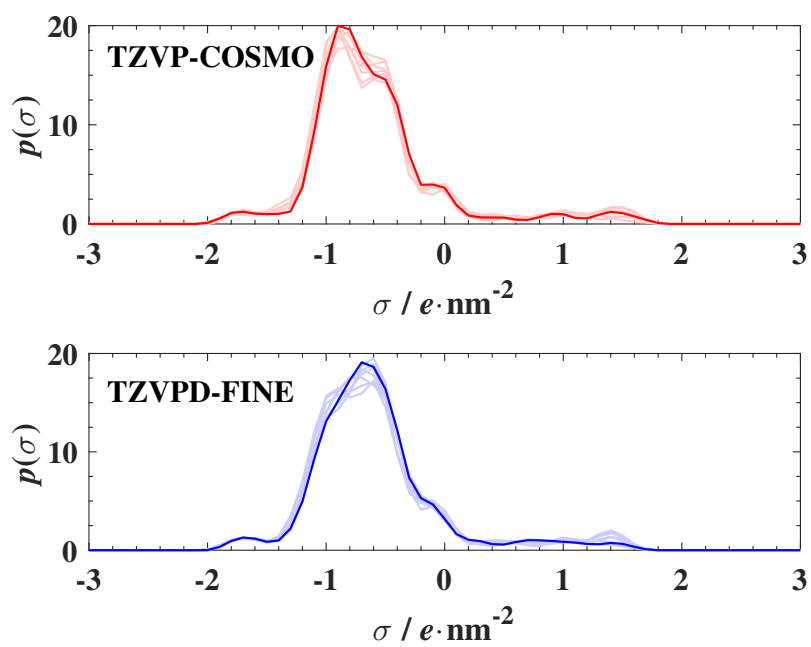


**Figure S75.**  $\sigma$ -profiles of N-20H, 3I, 1, 1 cation (abbreviations explained in the supplied Microsoft Excel spreadsheet, Table S1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).

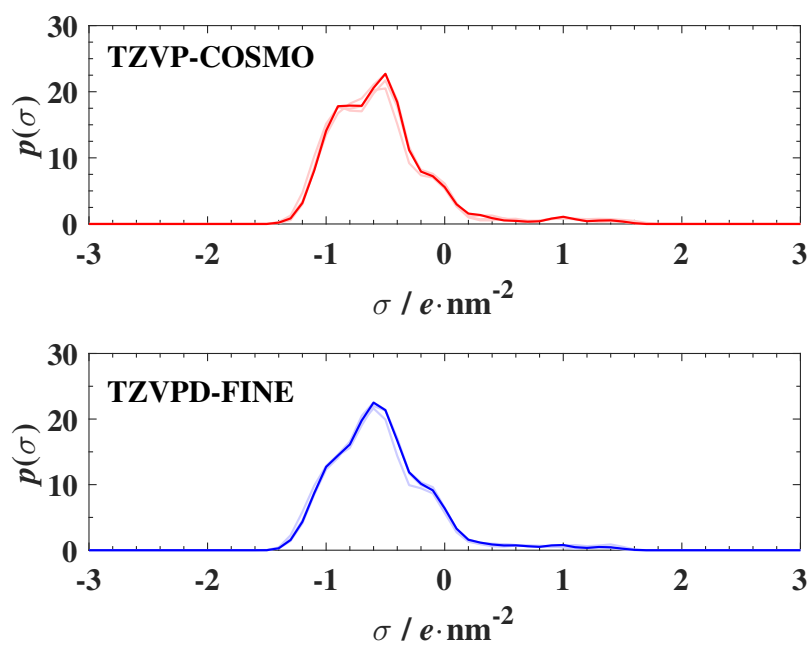


**Figure S76.**  $\sigma$ -profiles of N-20H, 1, 1, 1 cation (abbreviations explained in the supplied Microsoft Excel spreadsheet, Table S1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).

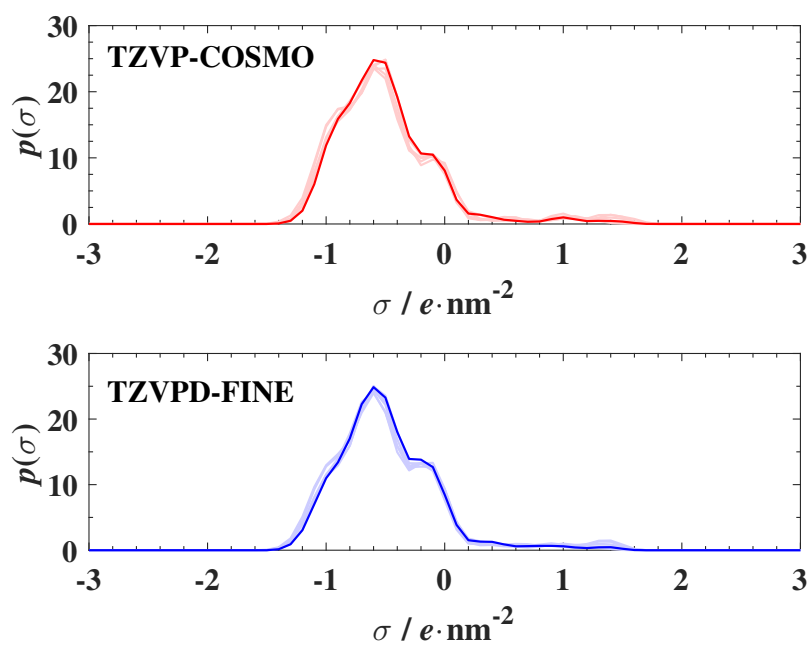




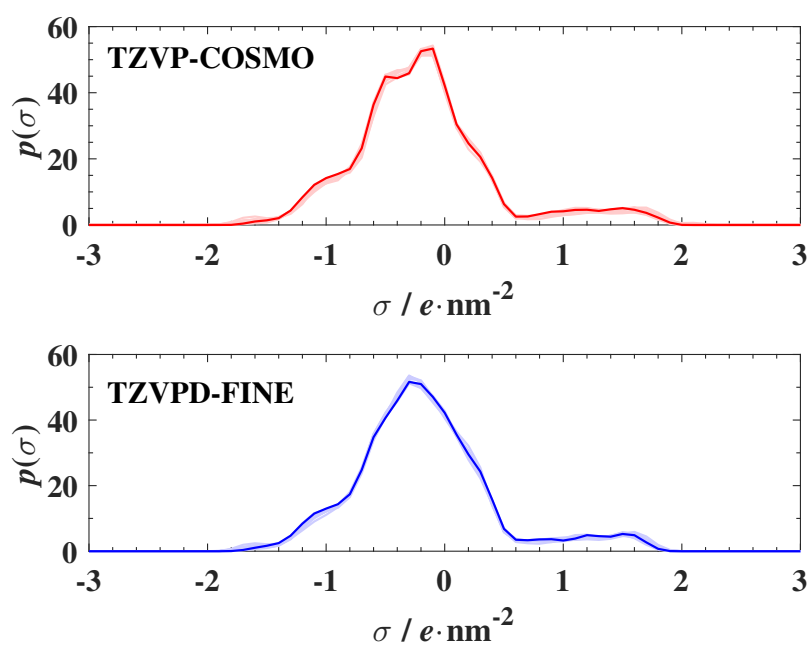
**Figure S77.**  $\sigma$ -profiles of N-20H, 2, 1, 1 cation (abbreviations explained in the supplied Microsoft Excel spreadsheet, Table S1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



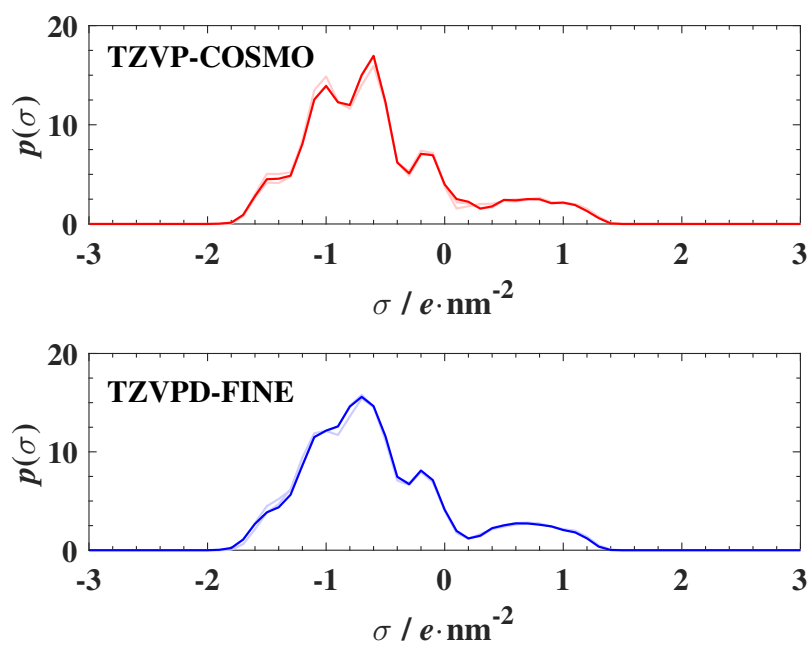
**Figure S78.**  $\sigma$ -profiles of N-201,2,1,1 cation (abbreviations explained in the supplied Microsoft Excel spreadsheet, Table S1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



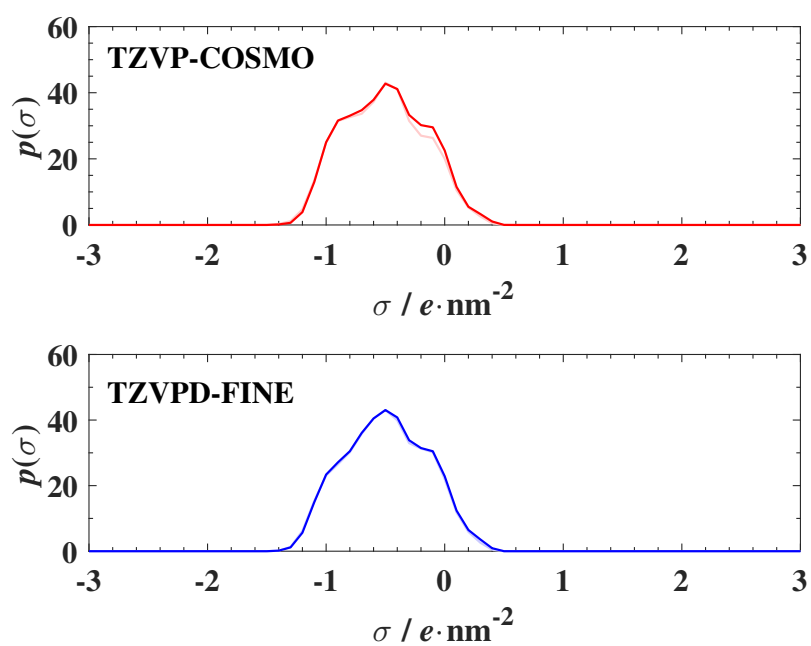
**Figure S79.**  $\sigma$ -profiles of N-201, 2, 2, 1 cation (abbreviations explained in the supplied Microsoft Excel spreadsheet, Table S1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



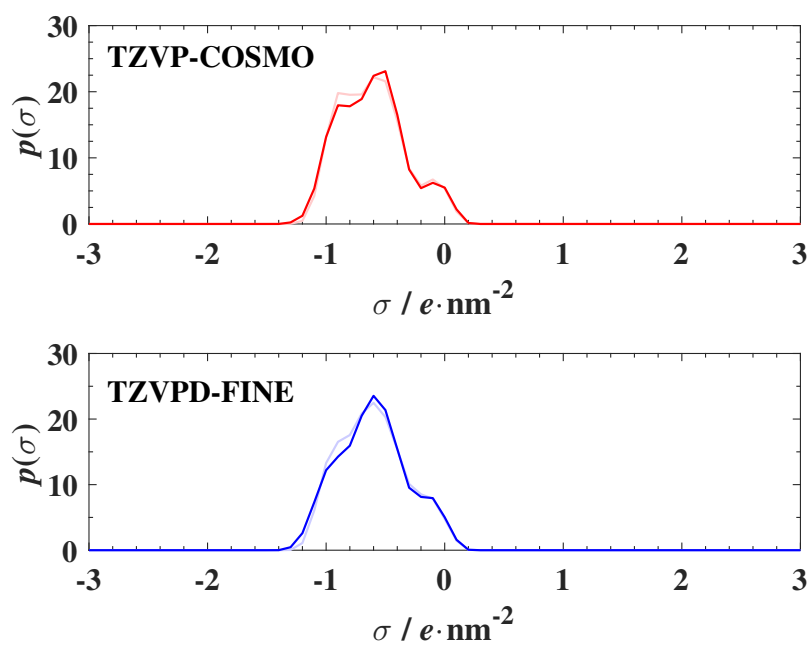
**Figure S80.**  $\sigma$ -profiles of N-2020H, [20]220H, 13, 1 cation (abbreviations explained in the supplied Microsoft Excel spreadsheet, Table S1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



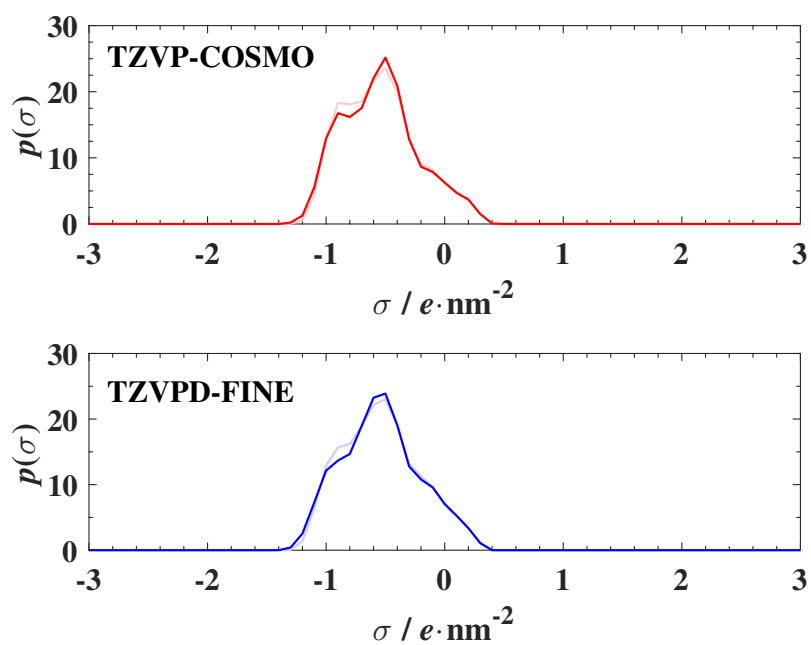
**Figure S81.**  $\sigma$ -profiles of N-1CN, 3I, 1, 1 cation (abbreviations explained in the supplied Microsoft Excel spreadsheet, Table S1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



**Figure S82.**  $\sigma$ -profiles of DC[N-3I, 1, 1]2-9 cation (abbreviations explained in the supplied Microsoft Excel spreadsheet, Table S1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).

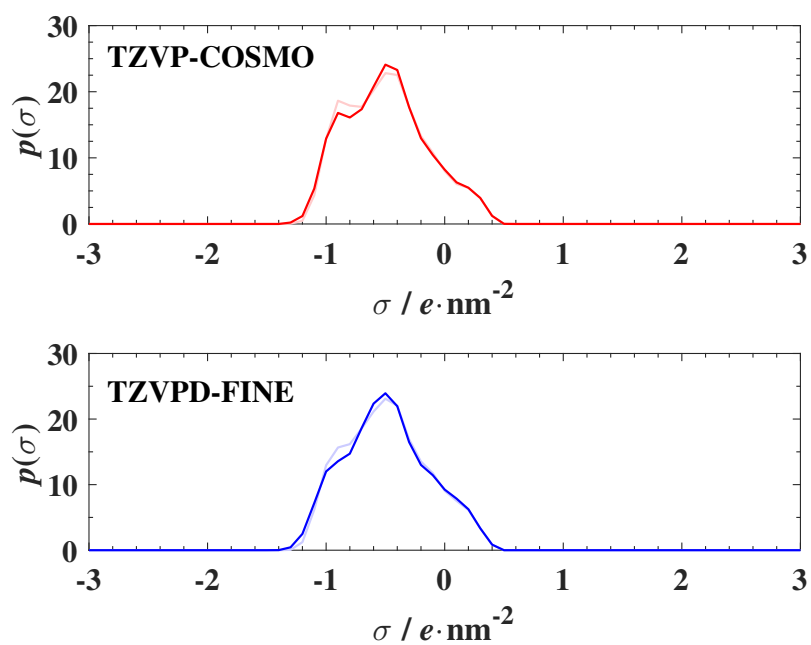


**Figure S83.**  $\sigma$ -profiles of PYR-2,1 cation (abbreviations explained in the supplied Microsoft Excel spreadsheet, Table S1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).

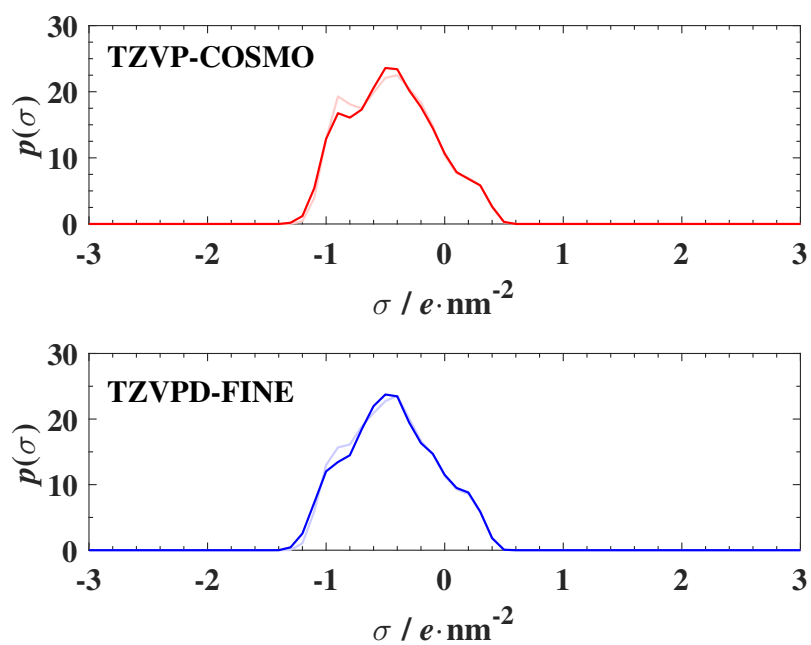


**Figure S84.**  $\sigma$ -profiles of PYR-3,1 cation (abbreviations explained in the supplied Microsoft Excel spreadsheet, Table S1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).

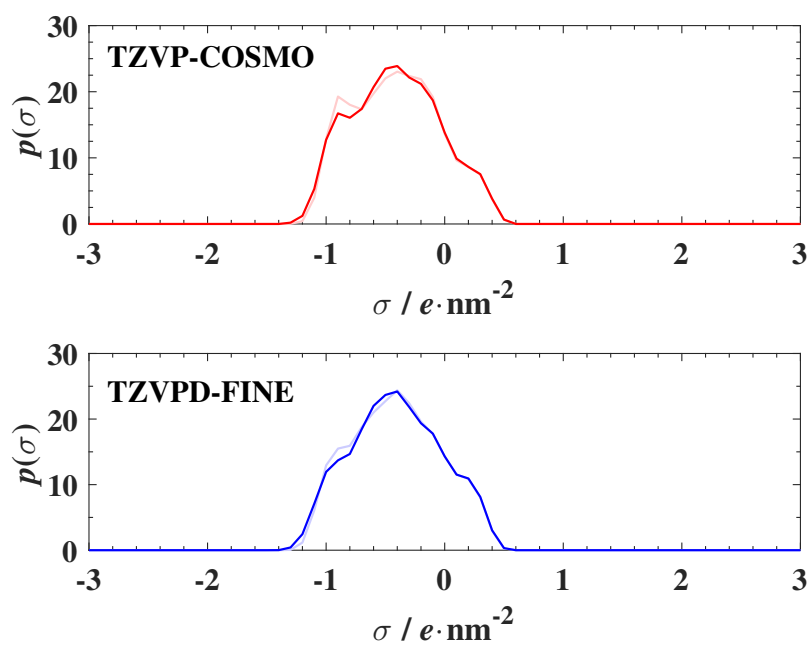




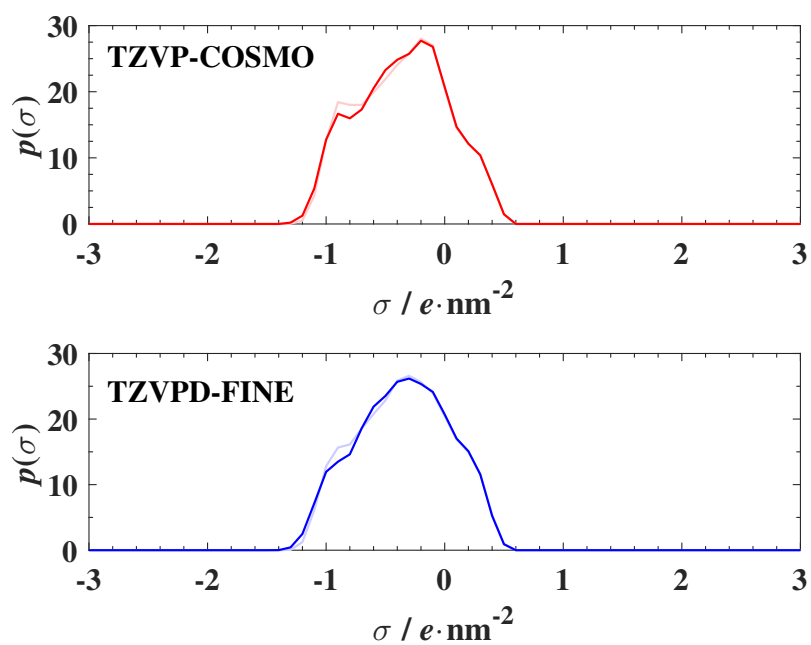
**Figure S85.**  $\sigma$ -profiles of PYR-4,1 cation (abbreviations explained in the supplied Microsoft Excel spreadsheet, Table S1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



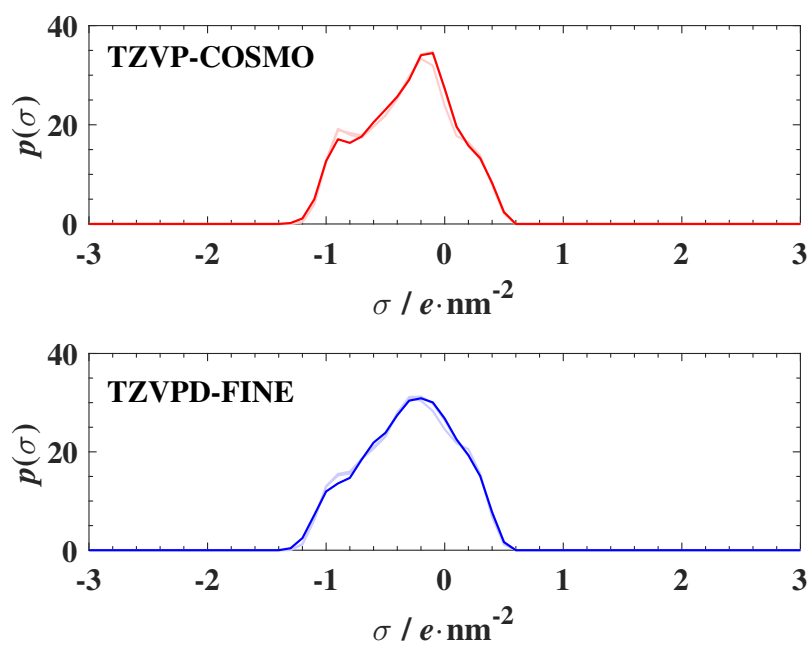
**Figure S86.**  $\sigma$ -profiles of PYR-5,1 cation (abbreviations explained in the supplied Microsoft Excel spreadsheet, Table S1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



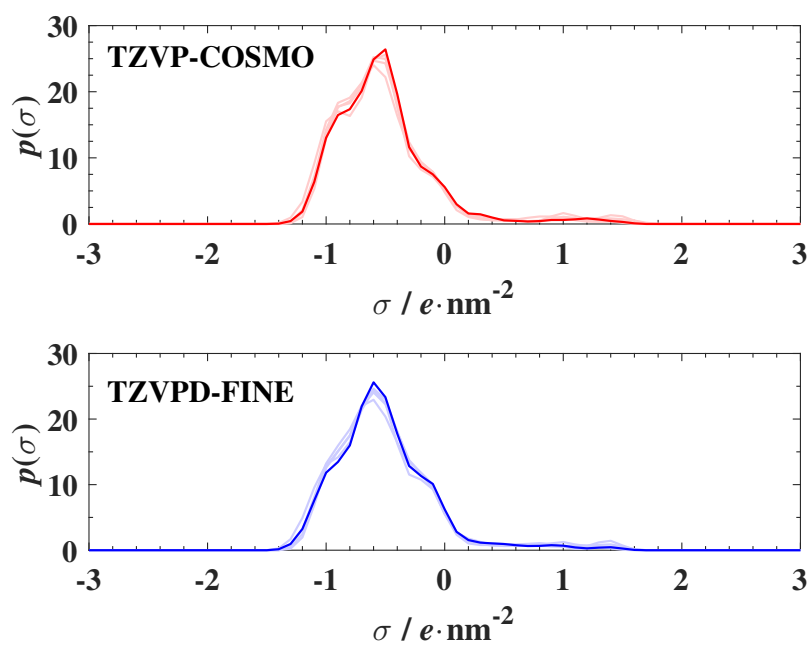
**Figure S87.**  $\sigma$ -profiles of PYR-6,1 cation (abbreviations explained in the supplied Microsoft Excel spreadsheet, Table S1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



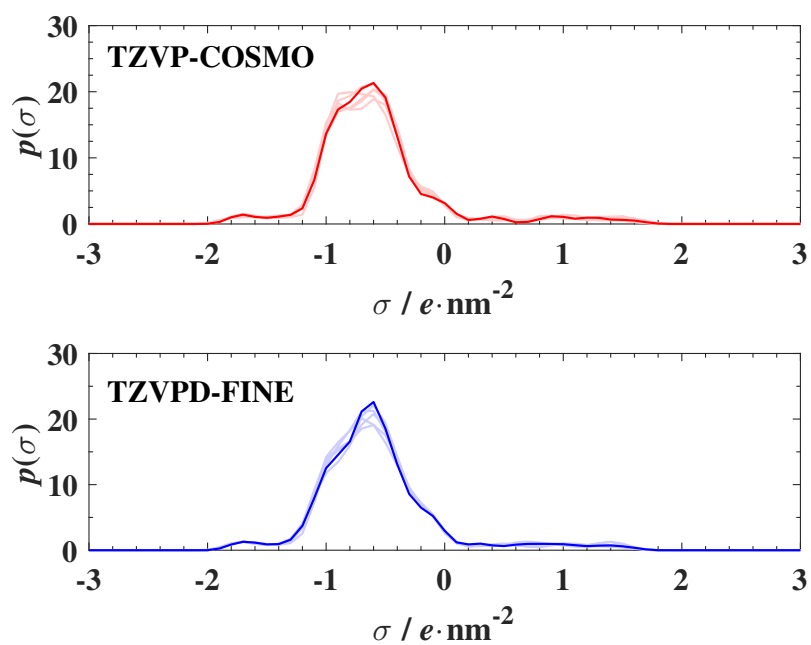
**Figure S88.**  $\sigma$ -profiles of PYR-8,1 cation (abbreviations explained in the supplied Microsoft Excel spreadsheet, Table S1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



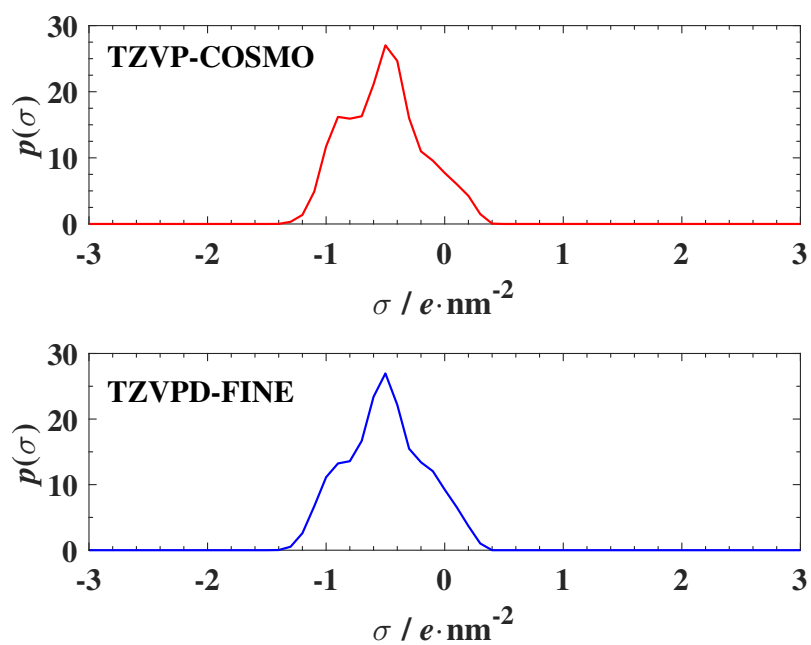
**Figure S89.**  $\sigma$ -profiles of PYR-10, 1 cation (abbreviations explained in the supplied Microsoft Excel spreadsheet, Table S1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



**Figure S90.**  $\sigma$ -profiles of PYR-201, 1 cation (abbreviations explained in the supplied Microsoft Excel spreadsheet, Table S1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).

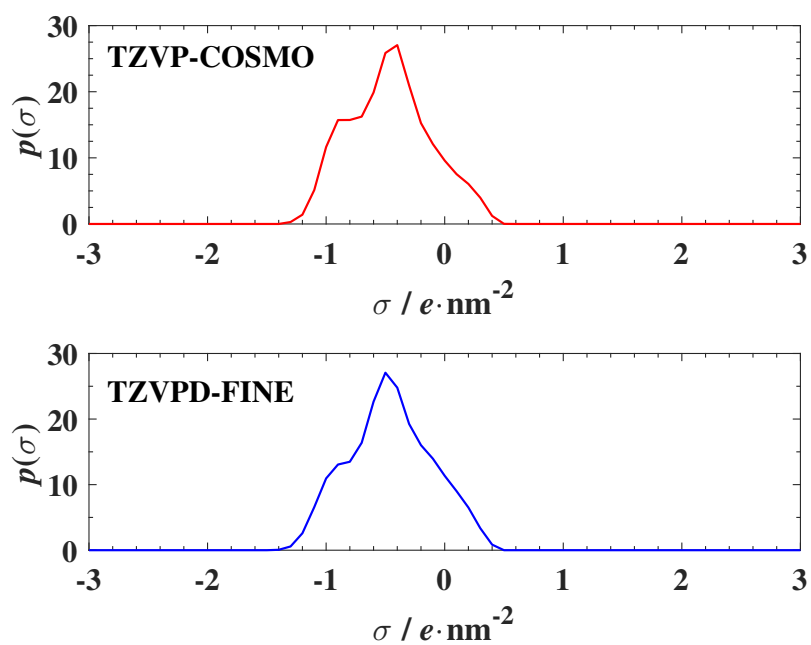


**Figure S91.**  $\sigma$ -profiles of PYR-20H, 1 cation (abbreviations explained in the supplied Microsoft Excel spreadsheet, Table S1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).

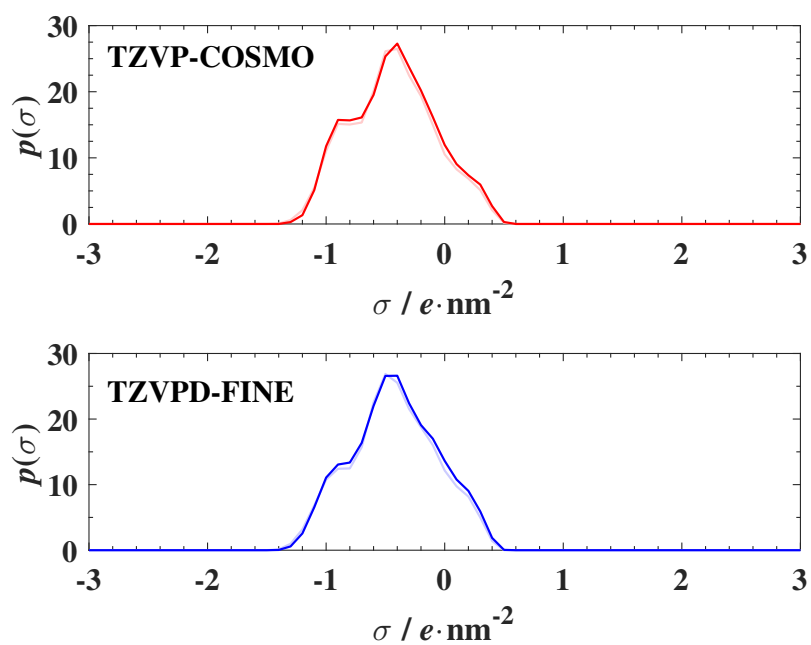


**Figure S92.**  $\sigma$ -profiles of PIP-3,1 cation (abbreviations explained in the supplied Microsoft Excel spreadsheet, Table S1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).

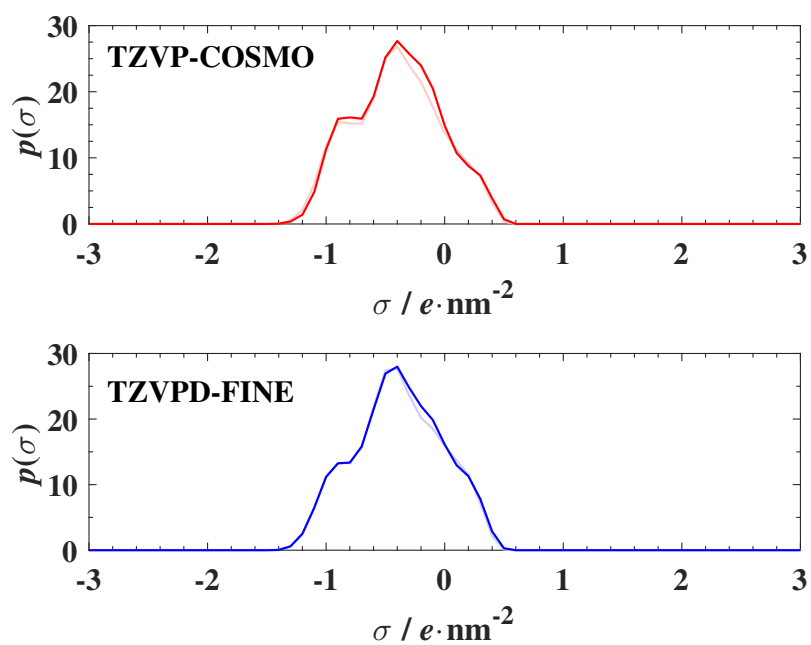




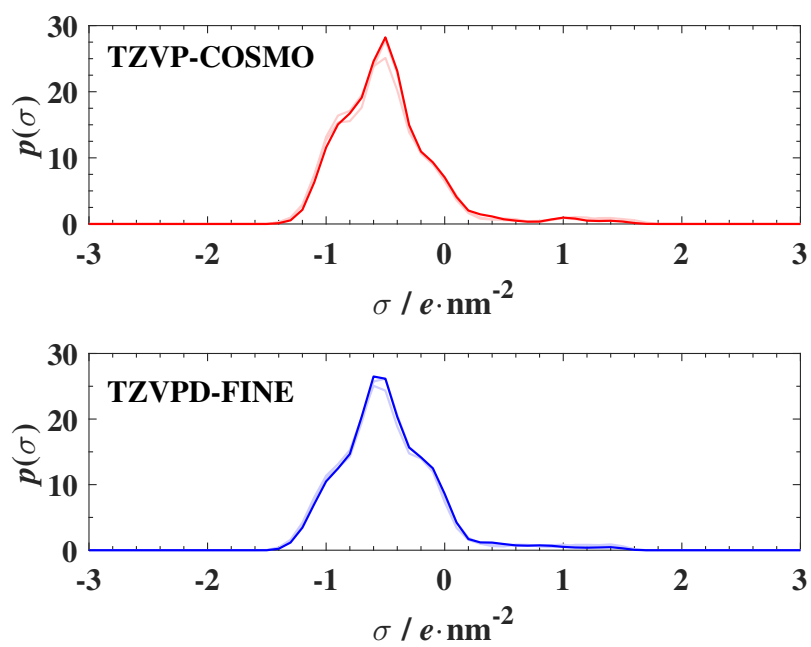
**Figure S93.**  $\sigma$ -profiles of PIP-4,1 cation (abbreviations explained in the supplied Microsoft Excel spreadsheet, Table S1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



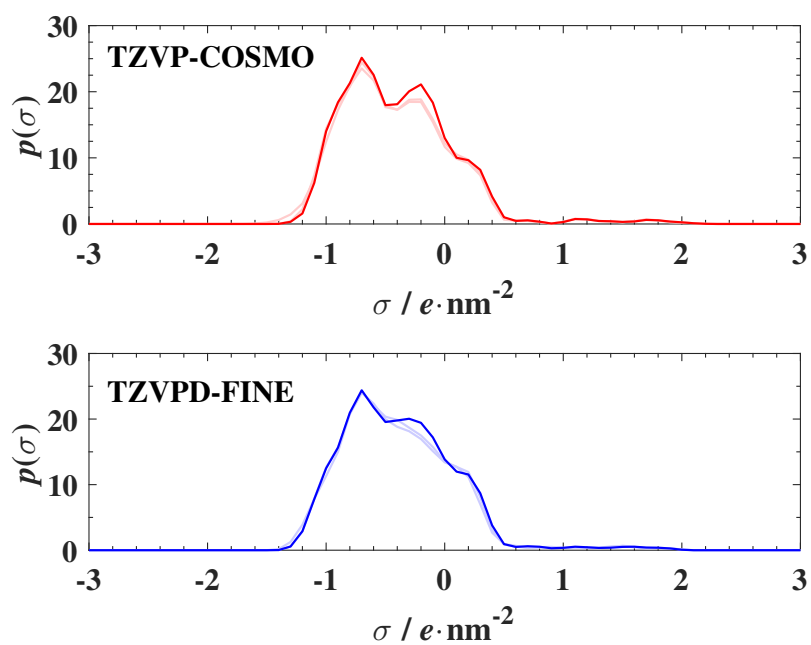
**Figure S94.**  $\sigma$ -profiles of PIP-5,1 cation (abbreviations explained in the supplied Microsoft Excel spreadsheet, Table S1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



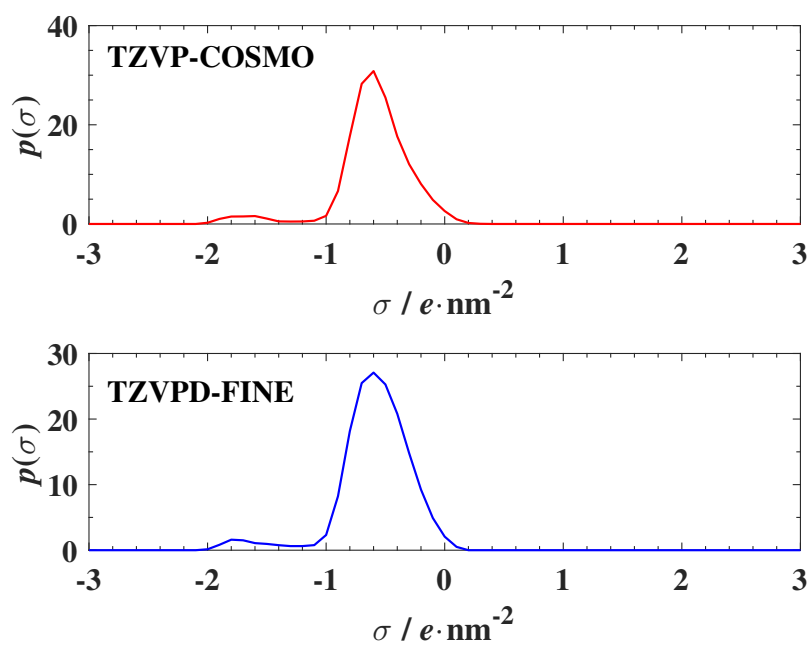
**Figure S95.**  $\sigma$ -profiles of PIP-6,1 cation (abbreviations explained in the supplied Microsoft Excel spreadsheet, Table S1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



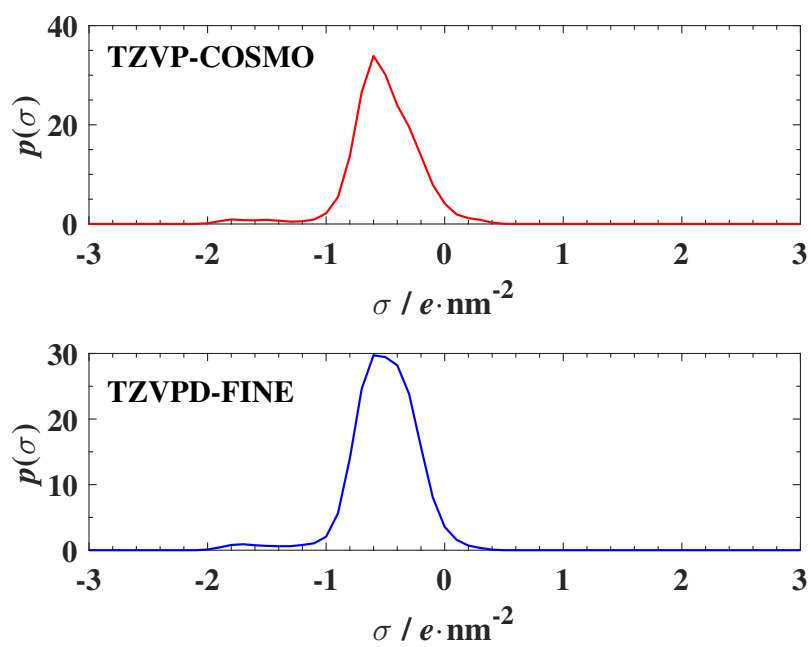
**Figure S96.**  $\sigma$ -profiles of PIP-201, 1 cation (abbreviations explained in the supplied Microsoft Excel spreadsheet, Table S1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



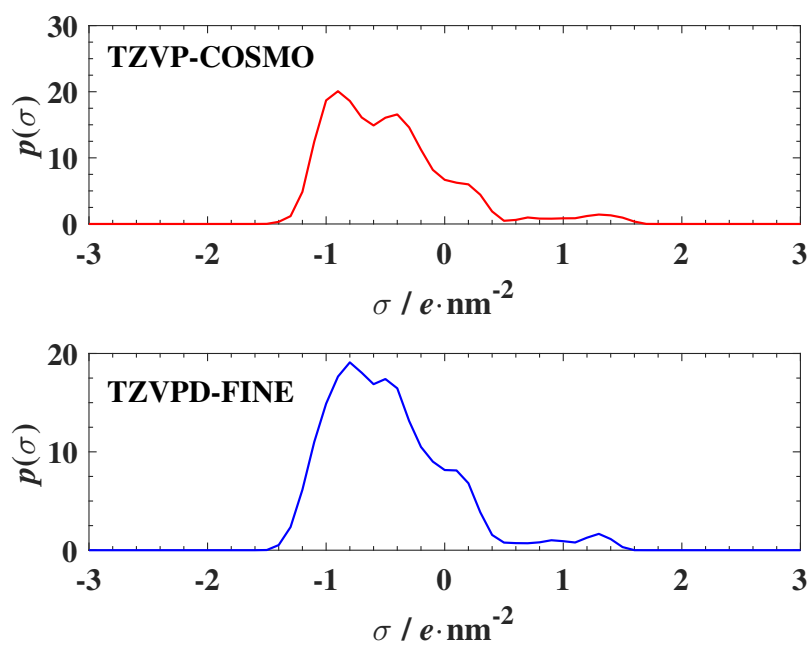
**Figure S97.**  $\sigma$ -profiles of DABCO-6 cation (abbreviations explained in the supplied Microsoft Excel spreadsheet, Table S1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



**Figure S98.**  $\sigma$ -profiles of DBNH cation (abbreviations explained in the supplied Microsoft Excel spreadsheet, Table S1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).

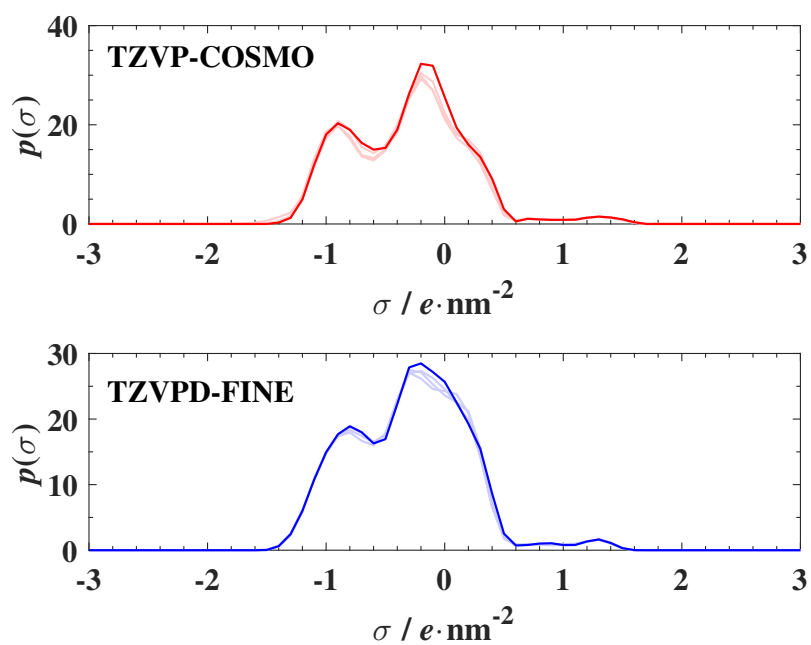


**Figure S99.**  $\sigma$ -profiles of TBDH-1 cation (abbreviations explained in the supplied Microsoft Excel spreadsheet, Table S1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).

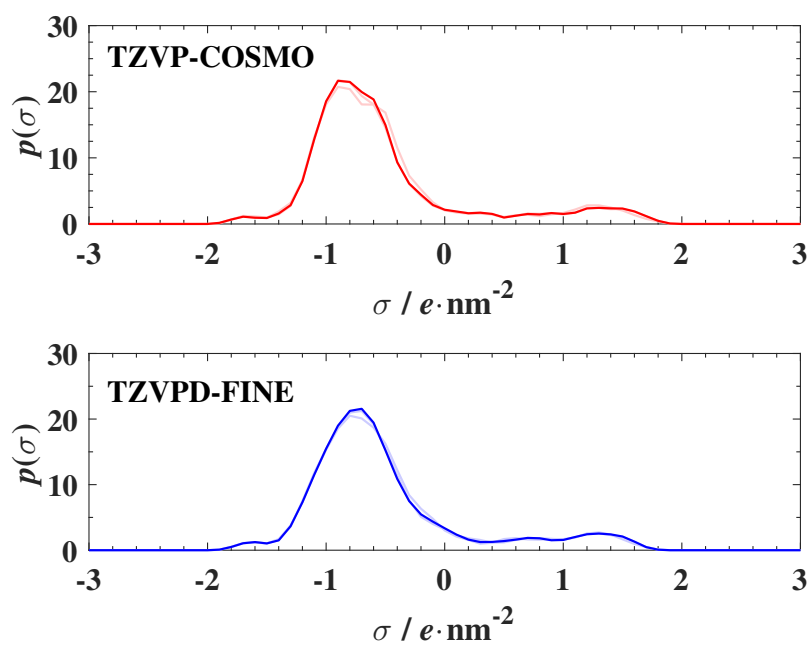


**Figure S100.**  $\sigma$ -profiles of MO-4,1 cation (abbreviations explained in the supplied Microsoft Excel spreadsheet, Table S1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).

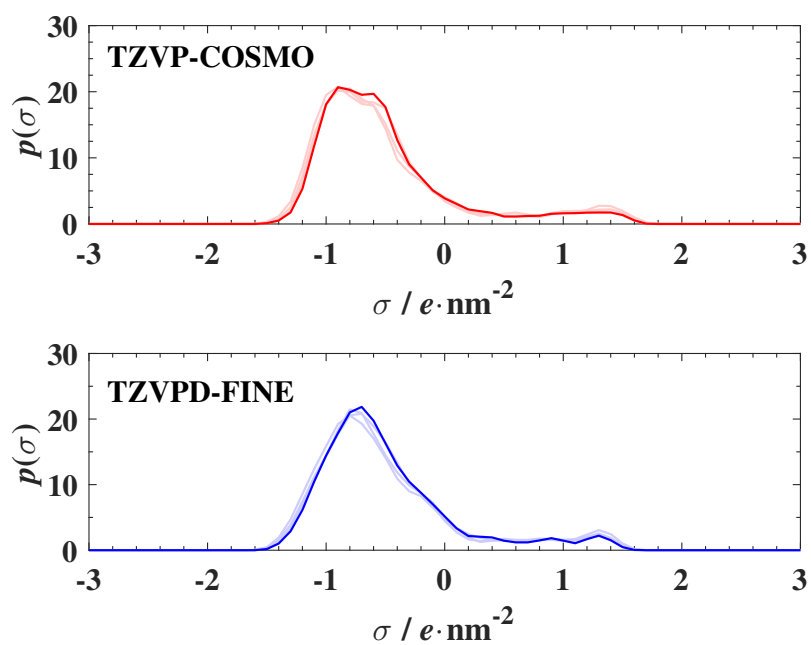




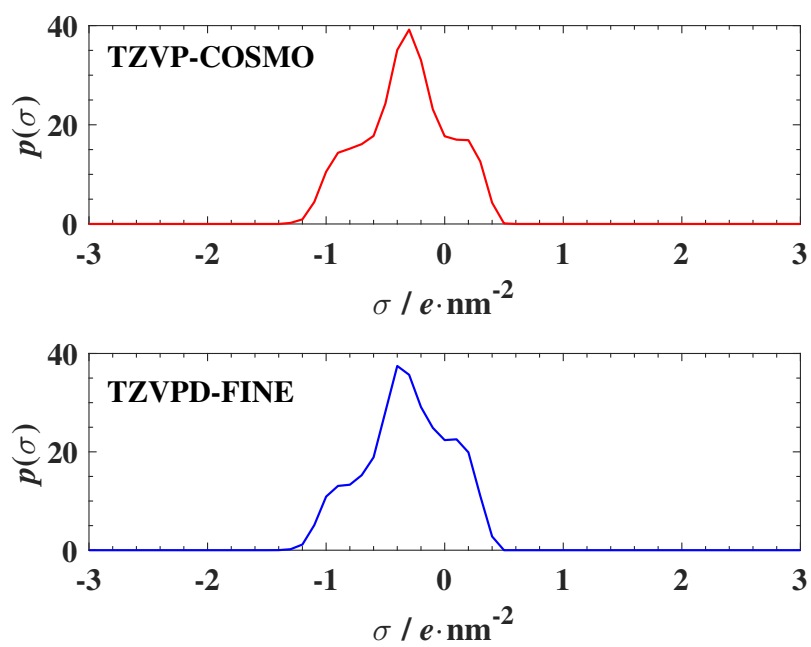
**Figure S101.**  $\sigma$ -profiles of M0-10, 1 cation (abbreviations explained in the supplied Microsoft Excel spreadsheet, Table S1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



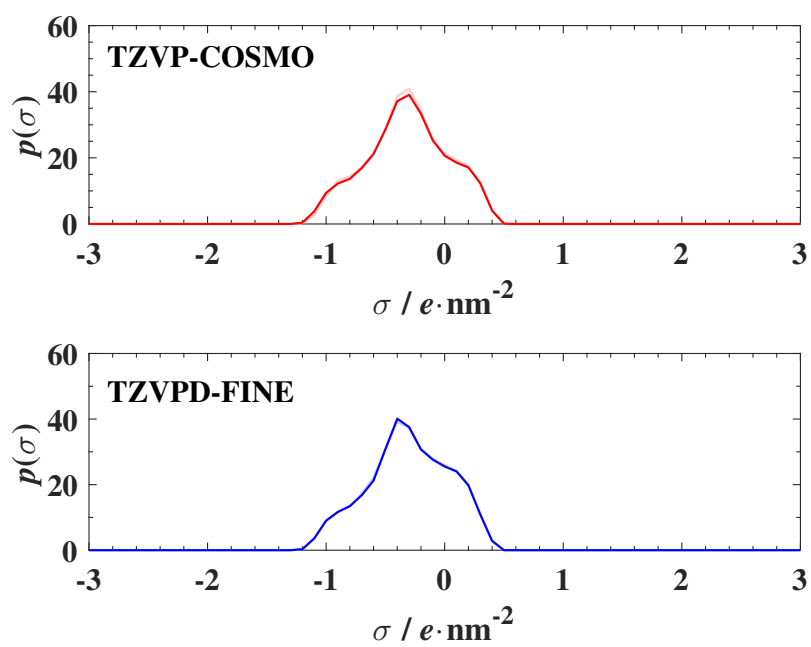
**Figure S102.**  $\sigma$ -profiles of MO-30H, 1 cation (abbreviations explained in the supplied Microsoft Excel spreadsheet, Table S1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



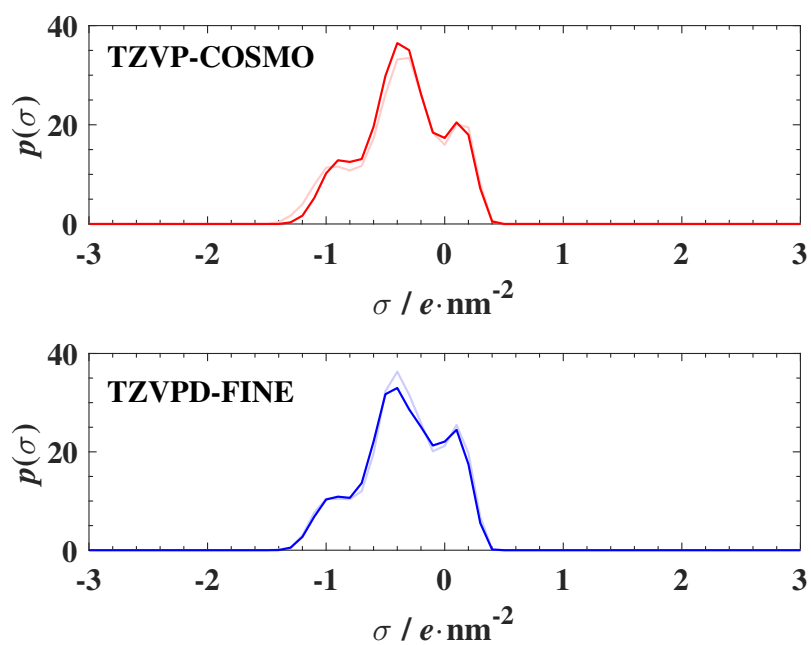
**Figure S103.**  $\sigma$ -profiles of M0-201, 1 cation (abbreviations explained in the supplied Microsoft Excel spreadsheet, Table S1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



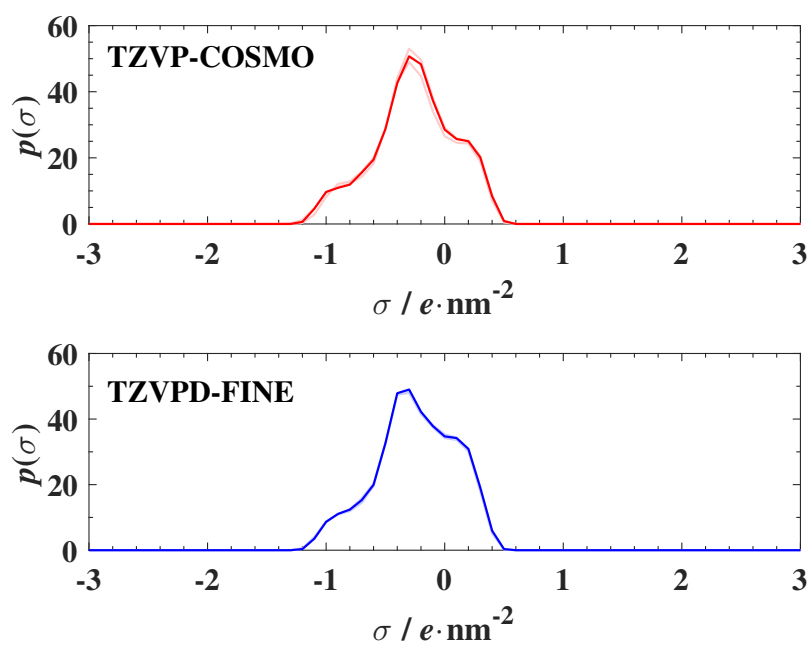
**Figure S104.**  $\sigma$ -profiles of P-4,4,4,1 cation (abbreviations explained in the supplied Microsoft Excel spreadsheet, Table S1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



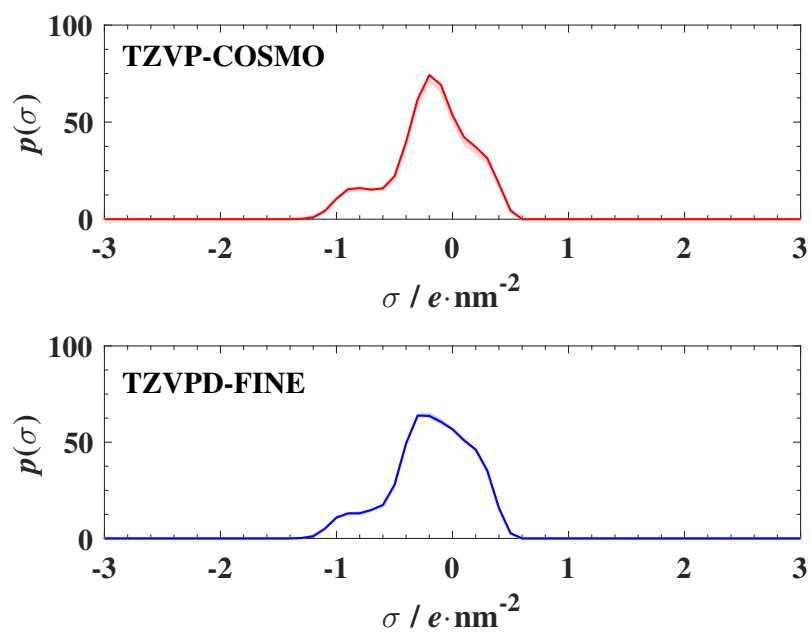
**Figure S105.**  $\sigma$ -profiles of P-4,4,4,2 cation (abbreviations explained in the supplied Microsoft Excel spreadsheet, Table S1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



**Figure S106.**  $\sigma$ -profiles of P-4I, 4I, 4I, 1 cation (abbreviations explained in the supplied Microsoft Excel spreadsheet, Table S1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).

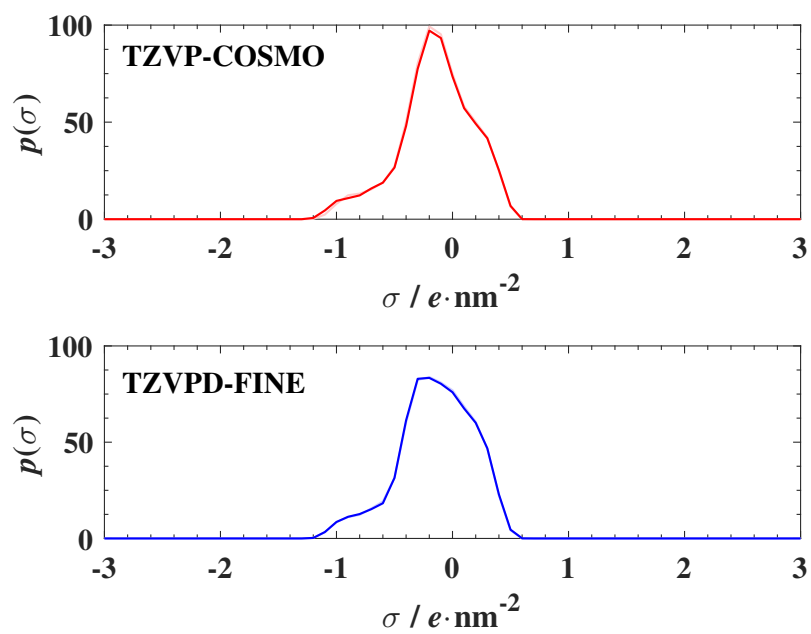


**Figure S107.**  $\sigma$ -profiles of P-6,4,4,4 cation (abbreviations explained in the supplied Microsoft Excel spreadsheet, Table S1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).

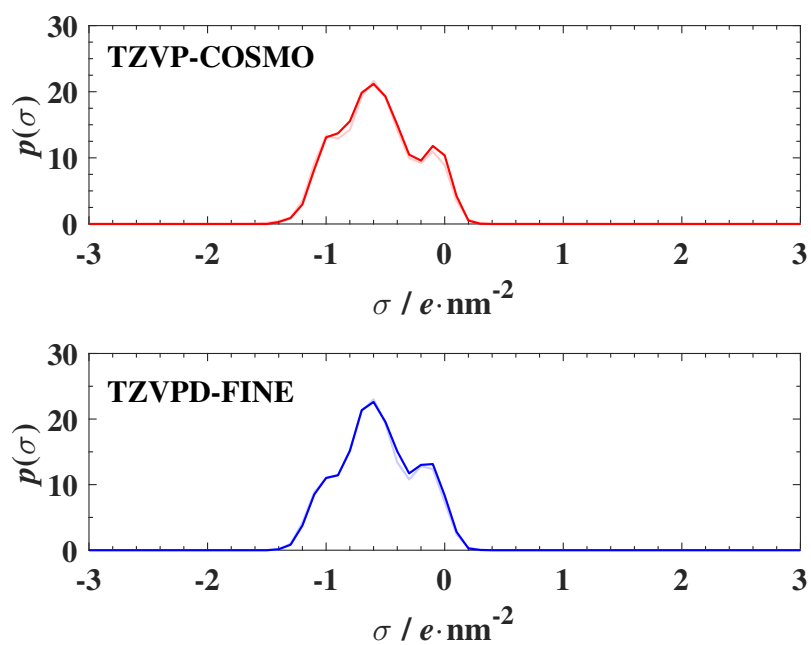


**Figure S108.**  $\sigma$ -profiles of P-8,8,8,1 cation (abbreviations explained in the supplied Microsoft Excel spreadsheet, Table S1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).

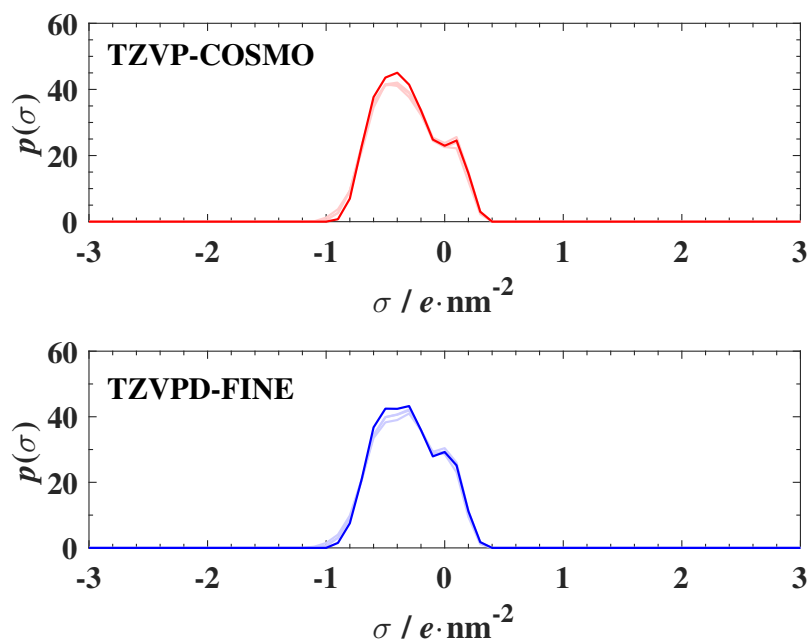




**Figure S109.**  $\sigma$ -profiles of P-14,6,6,6 cation (abbreviations explained in the supplied Microsoft Excel spreadsheet, Table S1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



**Figure S110.**  $\sigma$ -profiles of S-2, 2, 2 cation (abbreviations explained in the supplied Microsoft Excel spreadsheet, Table S1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).

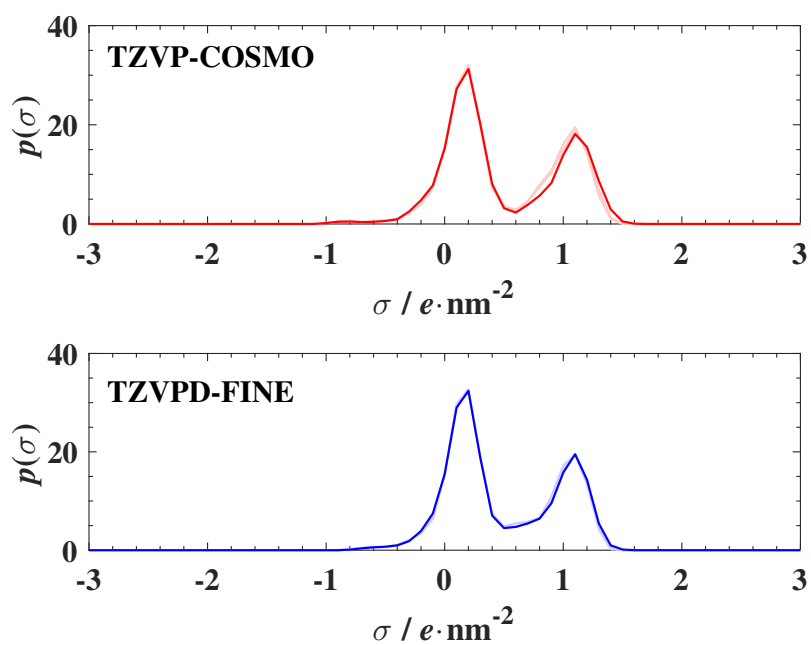


**Figure S111.**  $\sigma$ -profiles of CPROP-(N-2,2), (N-2,2), (N-2,2) cation (abbreviations explained in the supplied Microsoft Excel spreadsheet, Table S1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).

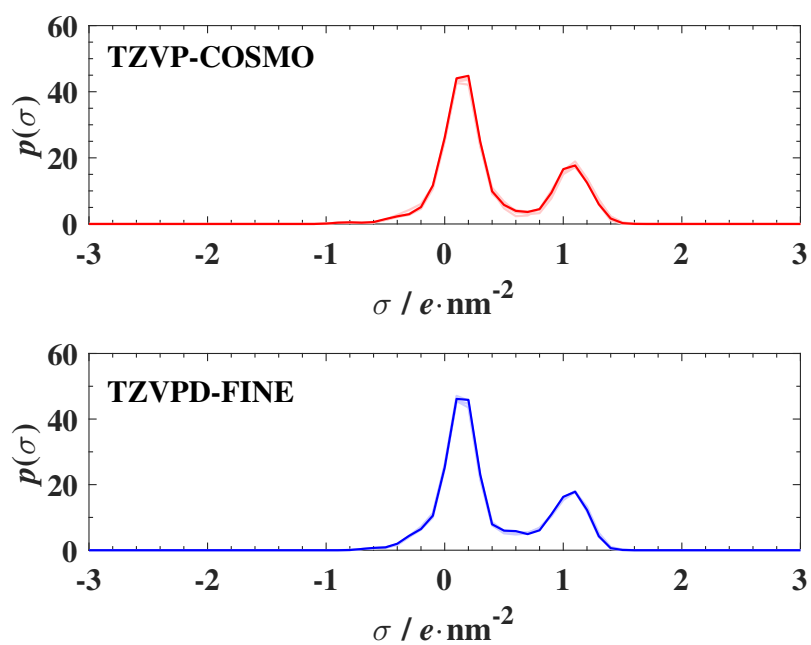
## 2 $\sigma$ -Profiles of Anions

S112 NTF2 . . . . .	117
S113 NPF2 . . . . .	118
S114 DCA . . . . .	119
S115 CCN3 . . . . .	120
S116 BF4 . . . . .	121
S117 BOB . . . . .	122
S118 TCB . . . . .	123
S119 PF6 . . . . .	124
S120 FAP . . . . .	125
S121 S03-1 . . . . .	126
S122 S03-PH1 . . . . .	127
S123 HS04 . . . . .	128
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S127 S04-8 . . . . .	132
S128 S04-201 . . . . .	133
S129 S04-202 . . . . .	134
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S133 P02-04,04 . . . . .	138
S134 P03H-1 . . . . .	139
S135 P03H-2 . . . . .	140
S136 P02-8I,8I . . . . .	141
S137 OTF . . . . .	142

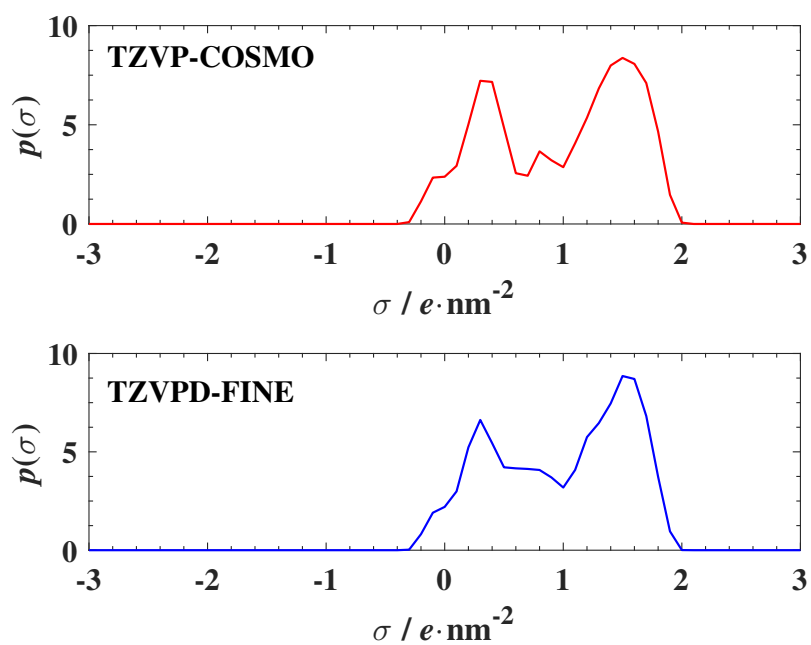
S138 FECL4 . . . . .	143
S139 COBR4 . . . . .	144
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S141 CL . . . . .	146
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S149 TFA . . . . .	154
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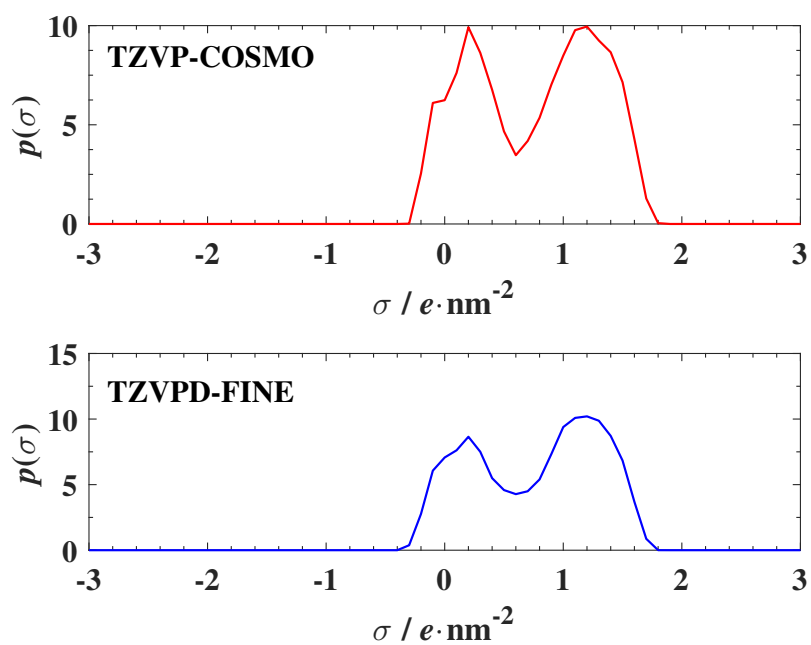
**Figure S112.**  $\sigma$ -profiles of NTF2 anion (abbreviations explained in the supplied Microsoft Excel spreadsheet, Table S1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



**Figure S113.**  $\sigma$ -profiles of NPF2 anion (abbreviations explained in the supplied Microsoft Excel spreadsheet, Table S1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).

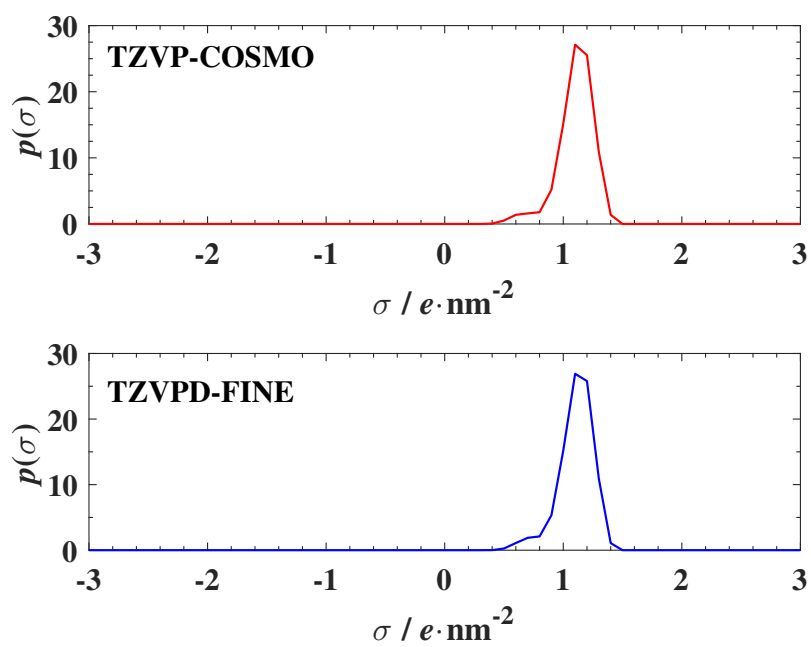


**Figure S114.**  $\sigma$ -profiles of DCA anion (abbreviations explained in the supplied Microsoft Excel spreadsheet, Table S1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).

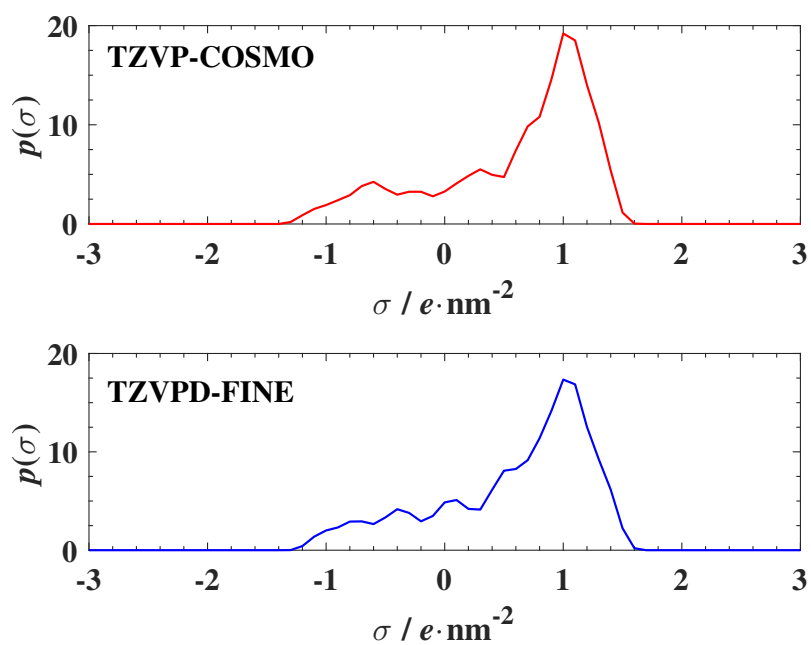


**Figure S115.**  $\sigma$ -profiles of CCN3 anion (abbreviations explained in the supplied Microsoft Excel spreadsheet, Table S1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).

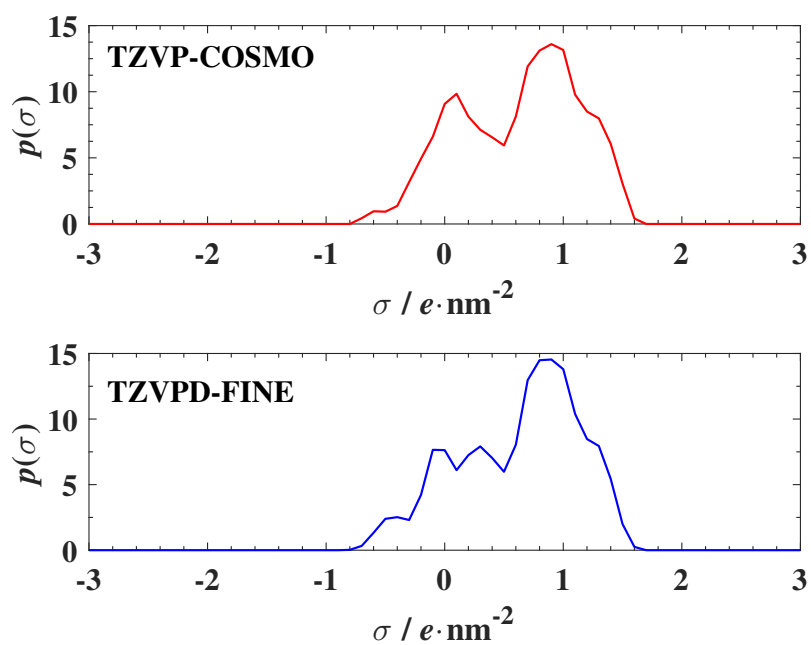




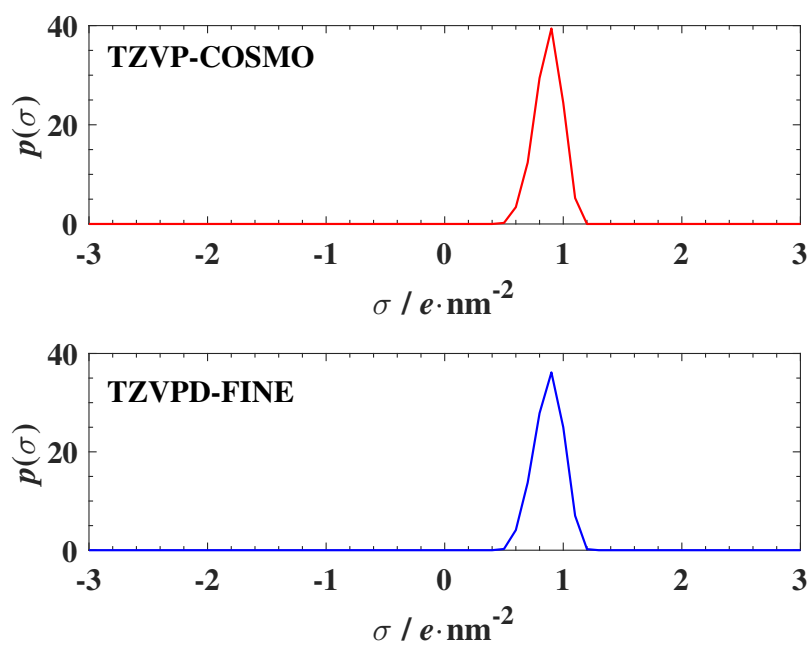
**Figure S116.**  $\sigma$ -profiles of  $\text{BF}_4$  anion (abbreviations explained in the supplied Microsoft Excel spreadsheet, Table S1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



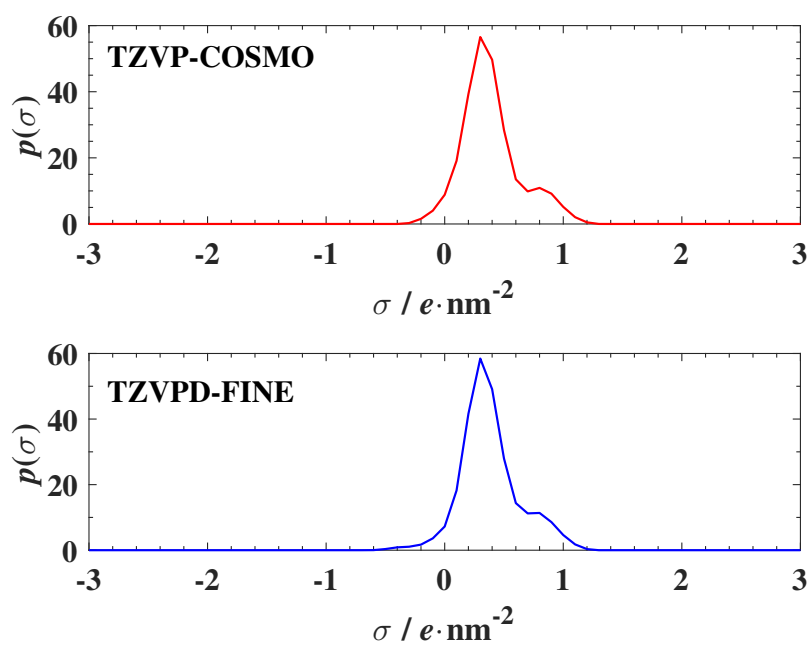
**Figure S117.**  $\sigma$ -profiles of BOB anion (abbreviations explained in the supplied Microsoft Excel spreadsheet, Table S1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



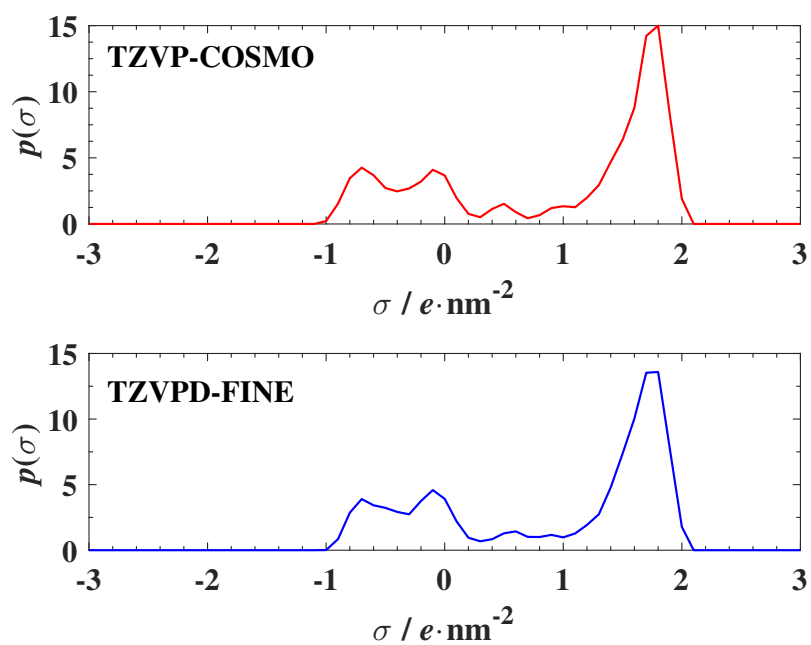
**Figure S118.**  $\sigma$ -profiles of TCB anion (abbreviations explained in the supplied Microsoft Excel spreadsheet, Table S1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



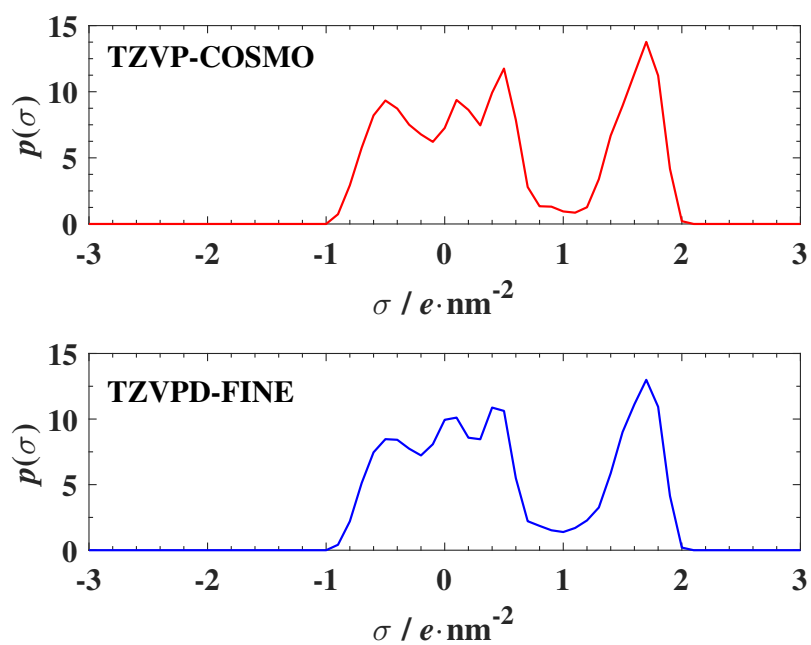
**Figure S119.**  $\sigma$ -profiles of PF6 anion (abbreviations explained in the supplied Microsoft Excel spreadsheet, Table S1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



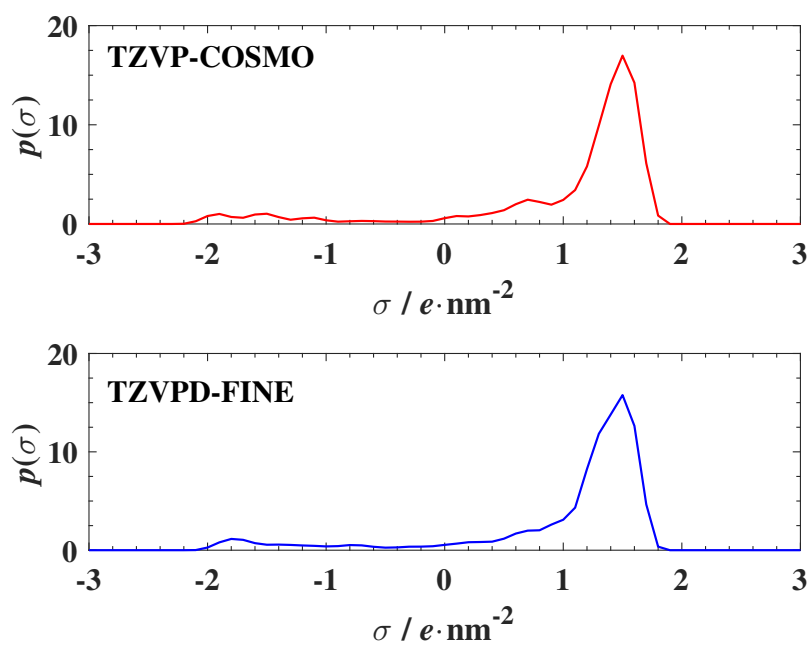
**Figure S120.**  $\sigma$ -profiles of FAP anion (abbreviations explained in the supplied Microsoft Excel spreadsheet, Table S1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



**Figure S121.**  $\sigma$ -profiles of S03-1 anion (abbreviations explained in the supplied Microsoft Excel spreadsheet, Table S1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).

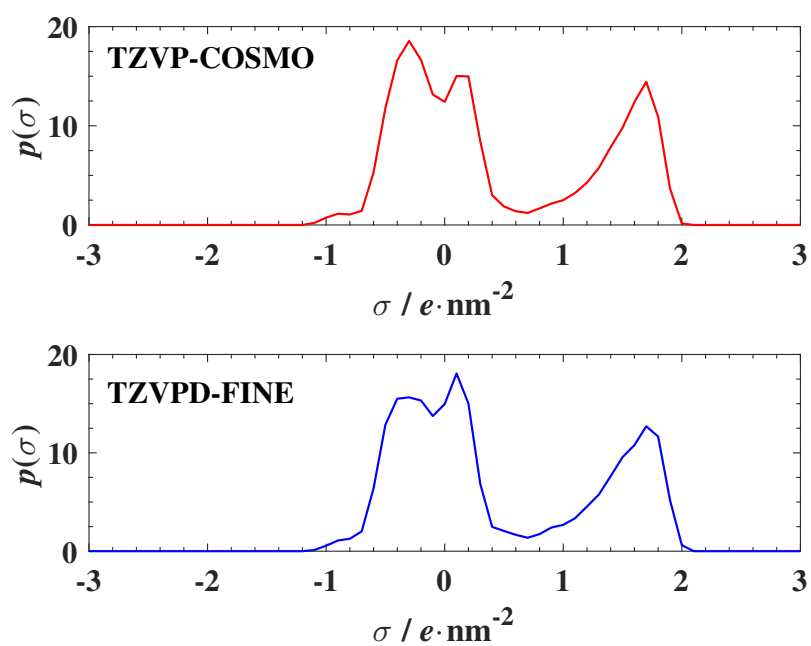


**Figure S122.**  $\sigma$ -profiles of S03-PH1 anion (abbreviations explained in the supplied Microsoft Excel spreadsheet, Table S1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).

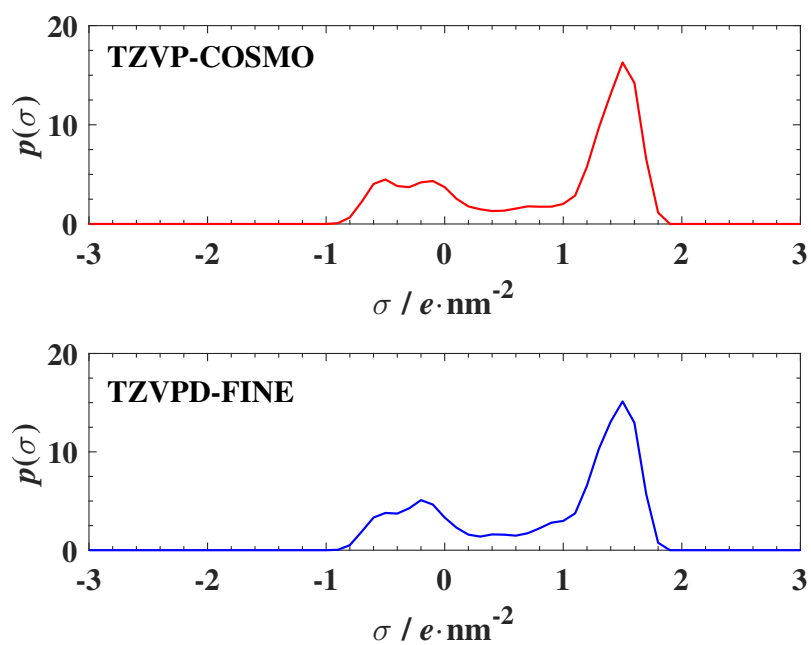


**Figure S123.**  $\sigma$ -profiles of HS04 anion (abbreviations explained in the supplied Microsoft Excel spreadsheet, Table S1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).

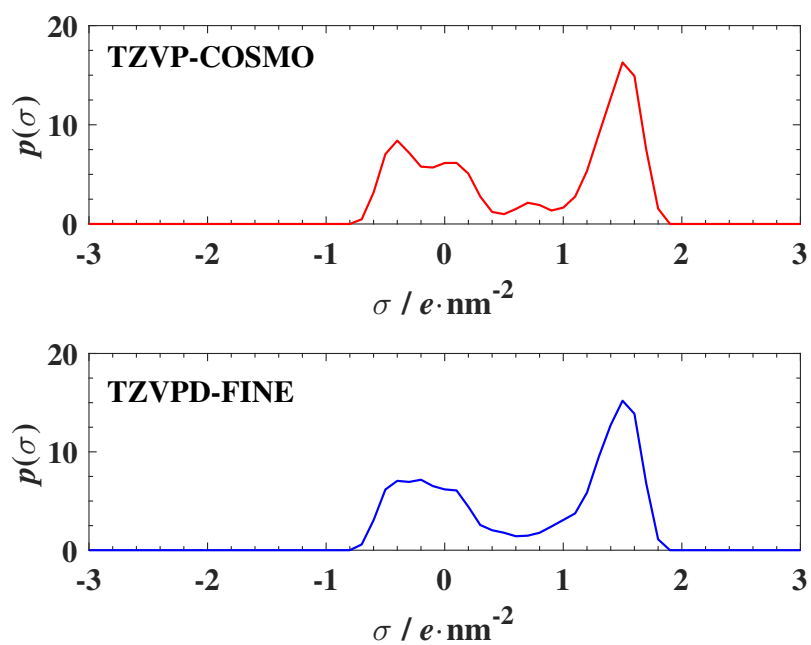




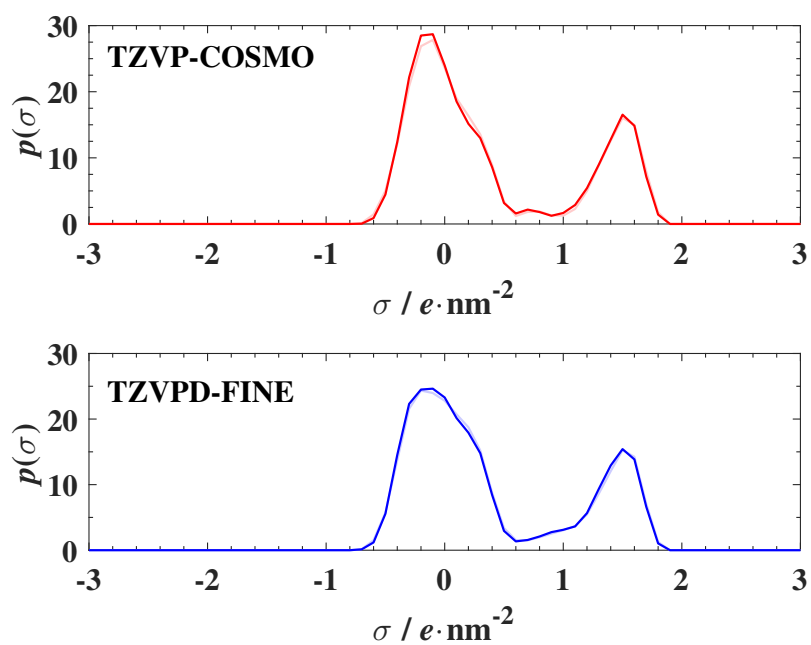
**Figure S124.**  $\sigma$ -profiles of CAMPHORSULFONATE anion (abbreviations explained in the supplied Microsoft Excel spreadsheet, Table S1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



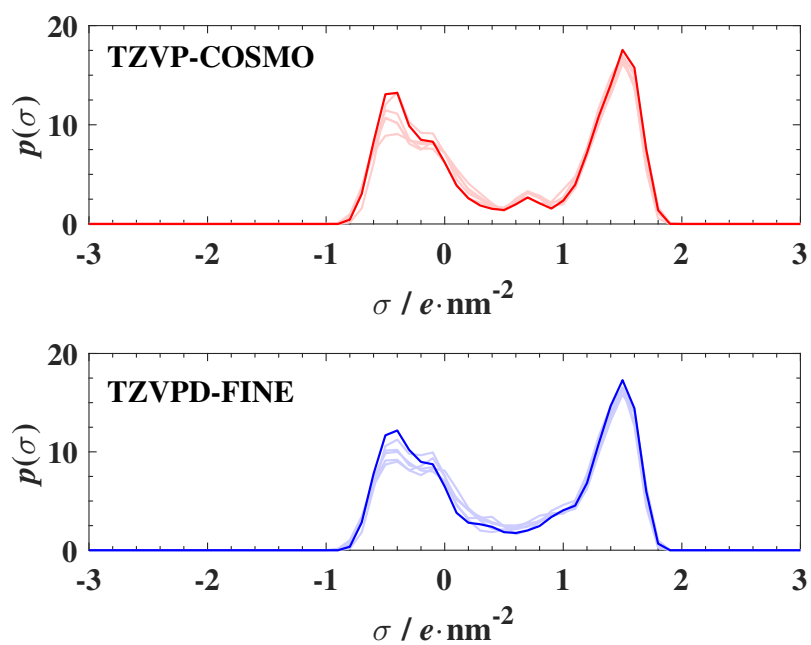
**Figure S125.**  $\sigma$ -profiles of S04-1 anion (abbreviations explained in the supplied Microsoft Excel spreadsheet, Table S1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



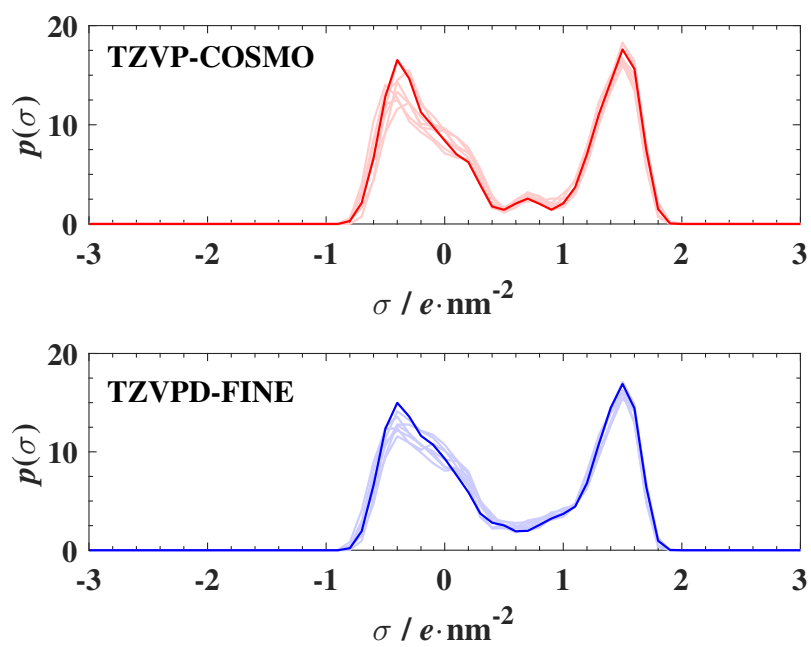
**Figure S126.**  $\sigma$ -profiles of S04-2 anion (abbreviations explained in the supplied Microsoft Excel spreadsheet, Table S1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



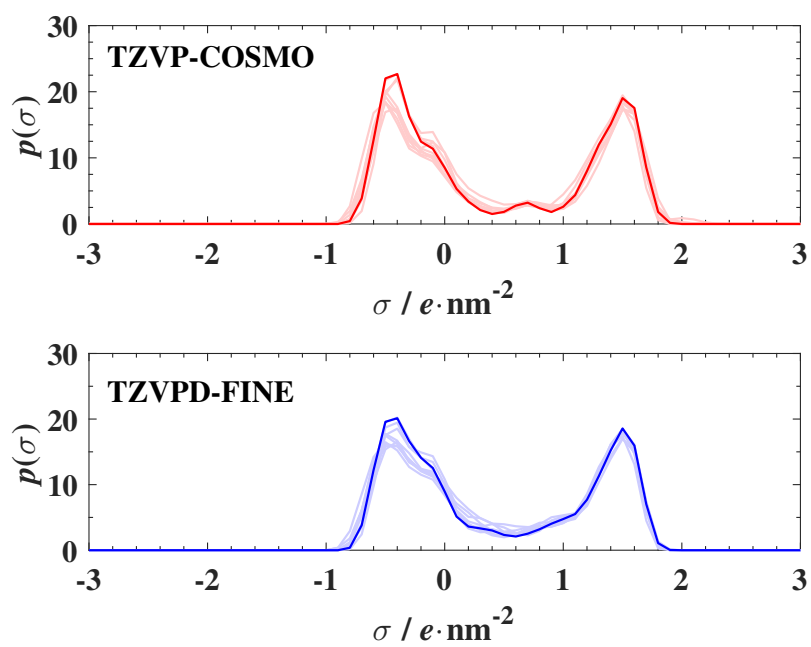
**Figure S127.**  $\sigma$ -profiles of S04-8 anion (abbreviations explained in the supplied Microsoft Excel spreadsheet, Table S1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



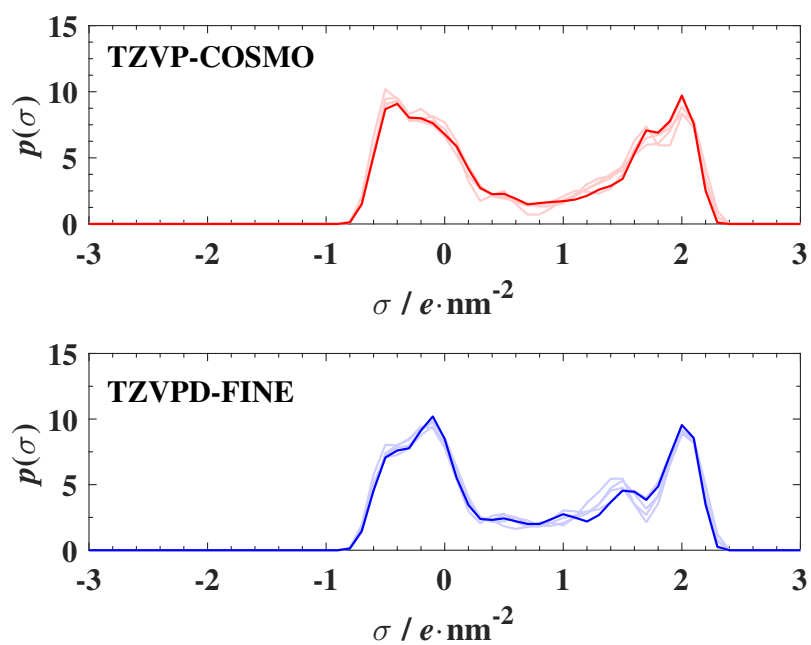
**Figure S128.**  $\sigma$ -profiles of S04-201 anion (abbreviations explained in the supplied Microsoft Excel spreadsheet, Table S1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



**Figure S129.**  $\sigma$ -profiles of S04-202 anion (abbreviations explained in the supplied Microsoft Excel spreadsheet, Table S1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).

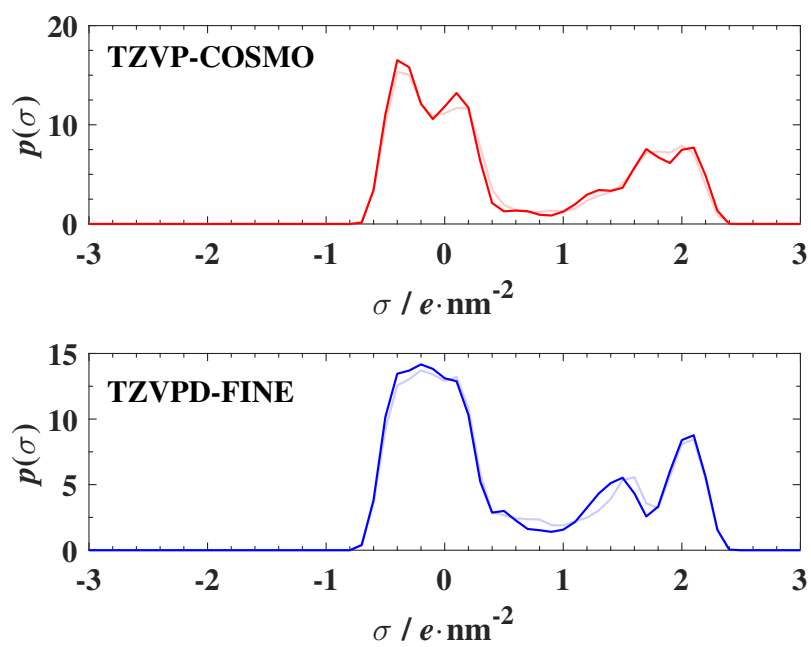


**Figure S130.**  $\sigma$ -profiles of S04-[20]21 anion (abbreviations explained in the supplied Microsoft Excel spreadsheet, Table S1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).

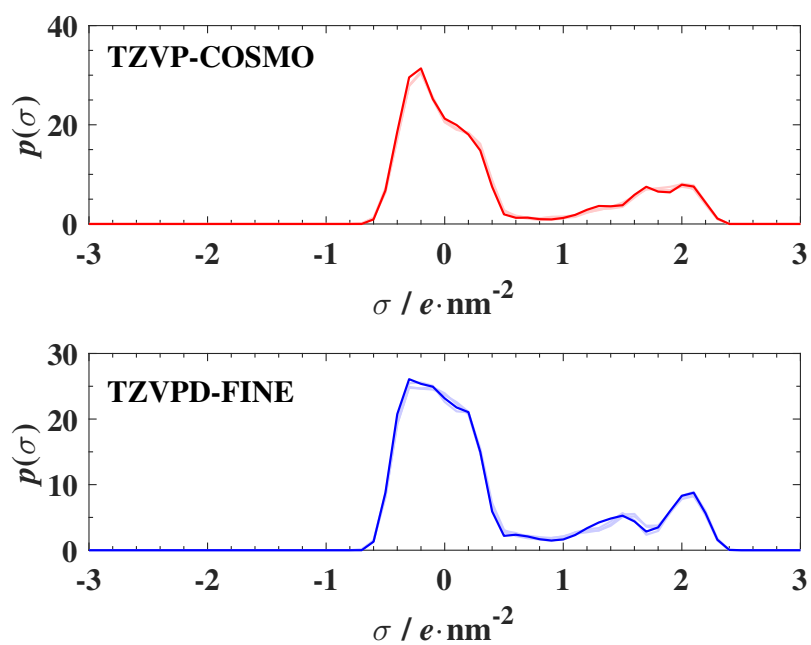


**Figure S131.**  $\sigma$ -profiles of P02-01, 01 anion (abbreviations explained in the supplied Microsoft Excel spreadsheet, Table S1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).

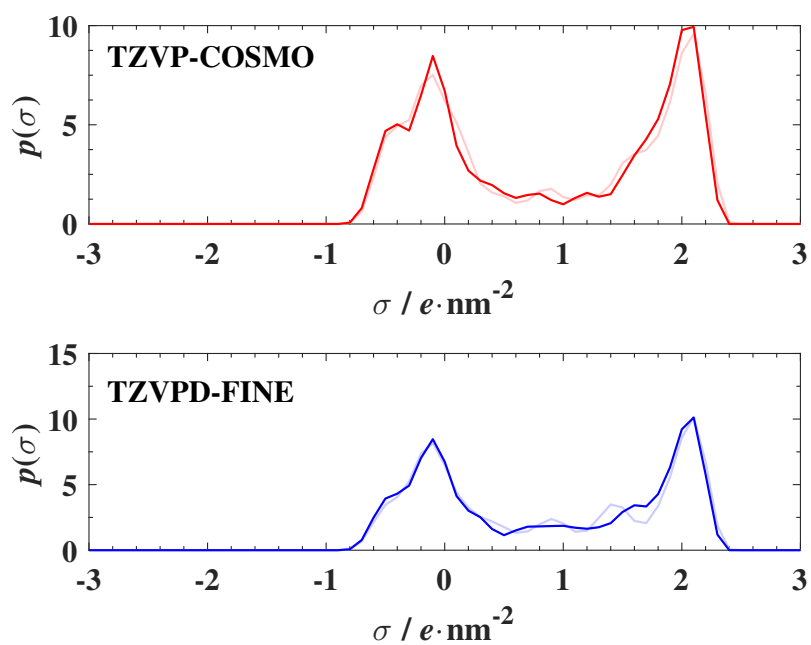




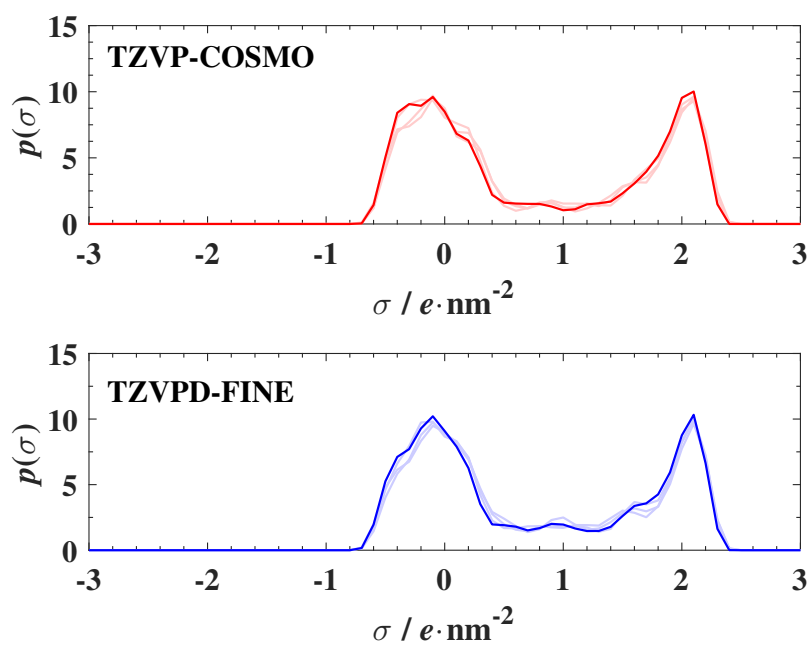
**Figure S132.**  $\sigma$ -profiles of P02-02,02 anion (abbreviations explained in the supplied Microsoft Excel spreadsheet, Table S1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



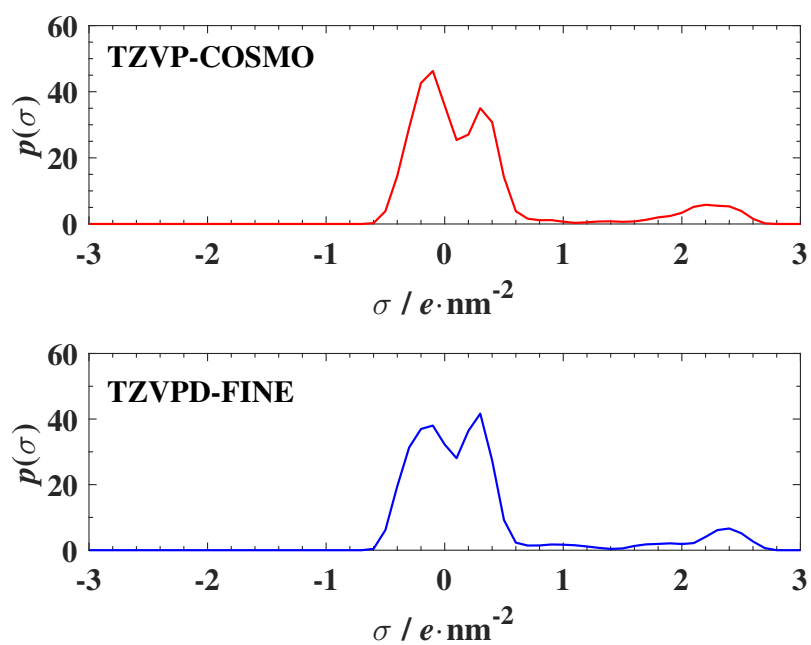
**Figure S133.**  $\sigma$ -profiles of P02-04, 04 anion (abbreviations explained in the supplied Microsoft Excel spreadsheet, Table S1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



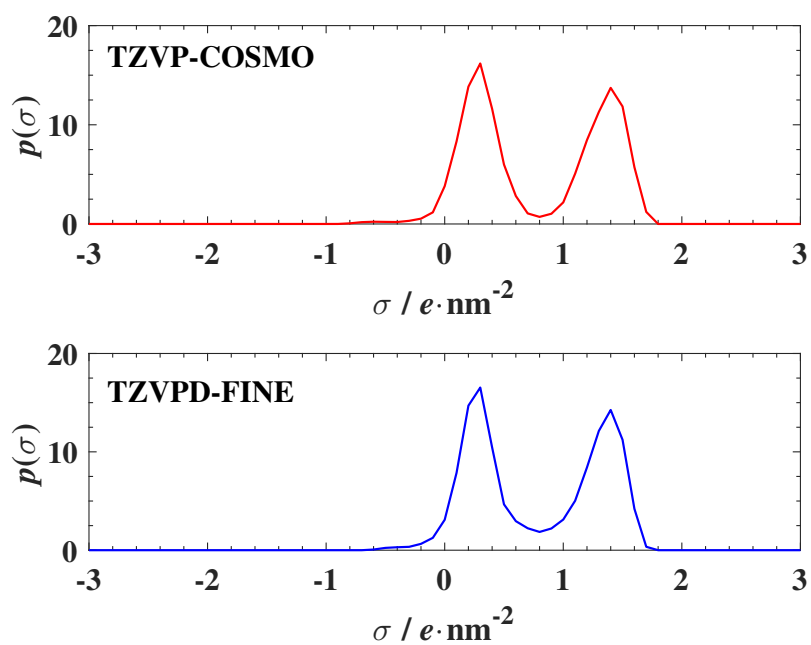
**Figure S134.**  $\sigma$ -profiles of P03H-1 anion (abbreviations explained in the supplied Microsoft Excel spreadsheet, Table S1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



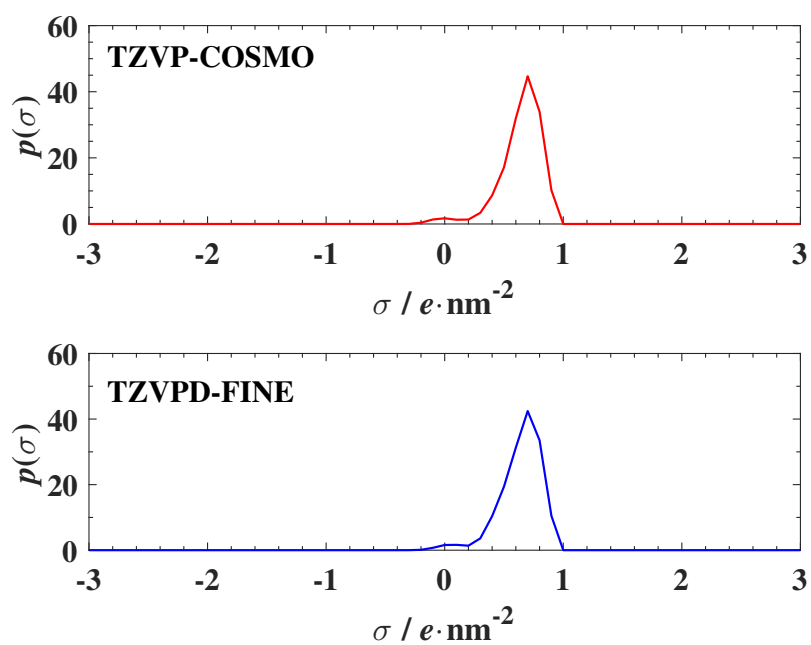
**Figure S135.**  $\sigma$ -profiles of P03H-2 anion (abbreviations explained in the supplied Microsoft Excel spreadsheet, Table S1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



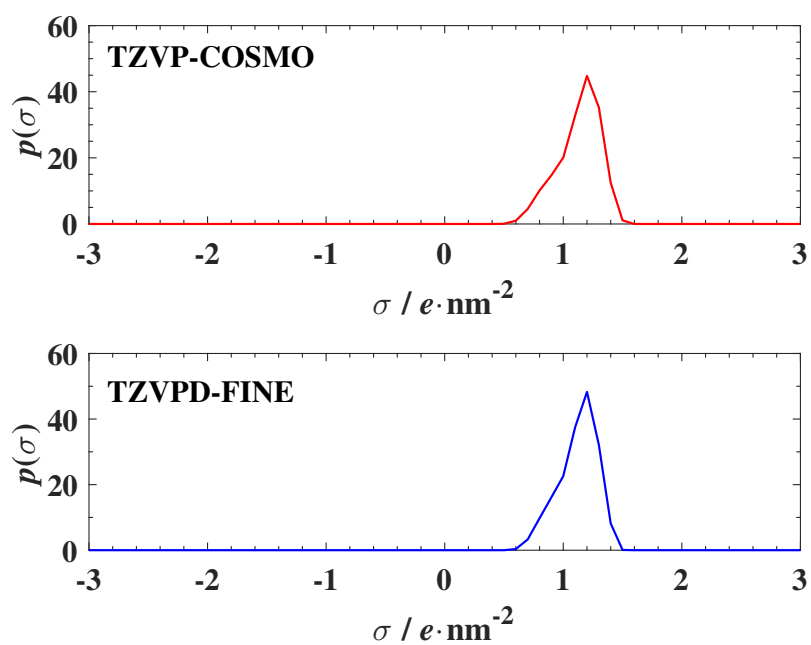
**Figure S136.**  $\sigma$ -profiles of P02-8I, 8I anion (abbreviations explained in the supplied Microsoft Excel spreadsheet, Table S1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



**Figure S137.**  $\sigma$ -profiles of OTF anion (abbreviations explained in the supplied Microsoft Excel spreadsheet, Table S1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).

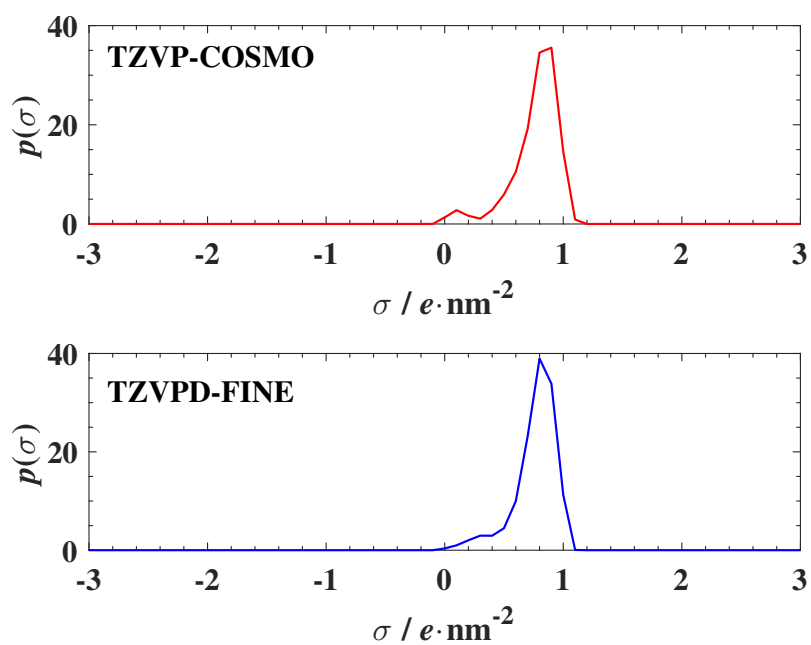


**Figure S138.**  $\sigma$ -profiles of FECL4 anion (abbreviations explained in the supplied Microsoft Excel spreadsheet, Table S1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).

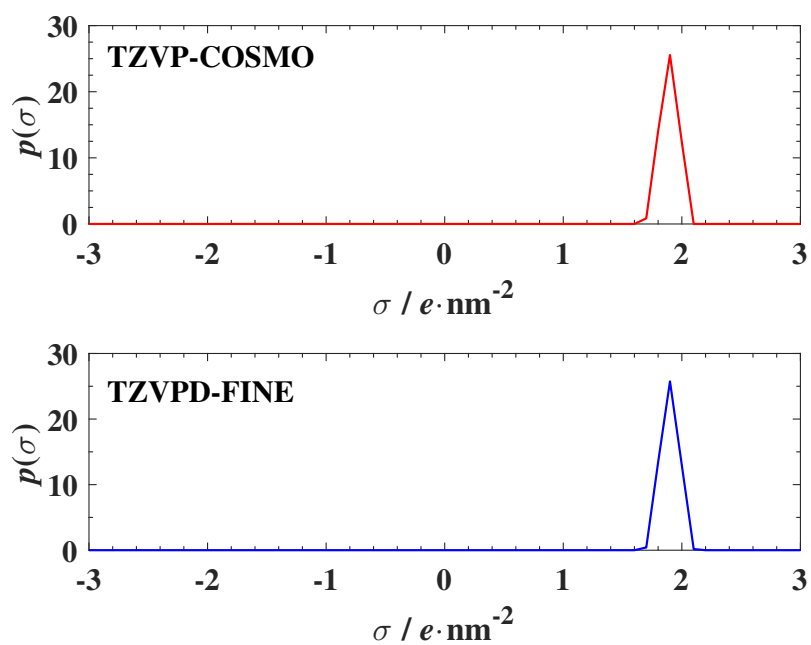


**Figure S139.**  $\sigma$ -profiles of COBR4 anion (abbreviations explained in the supplied Microsoft Excel spreadsheet, Table S1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).

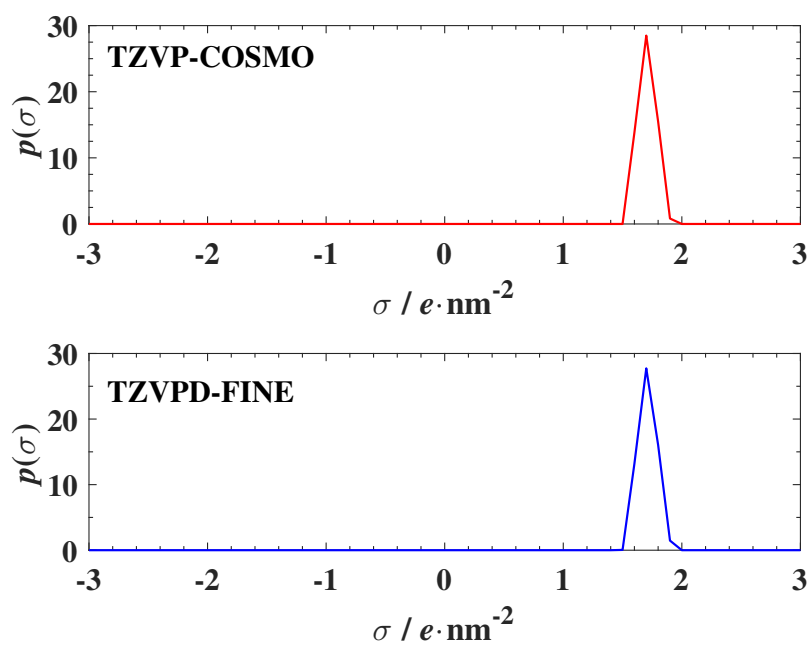




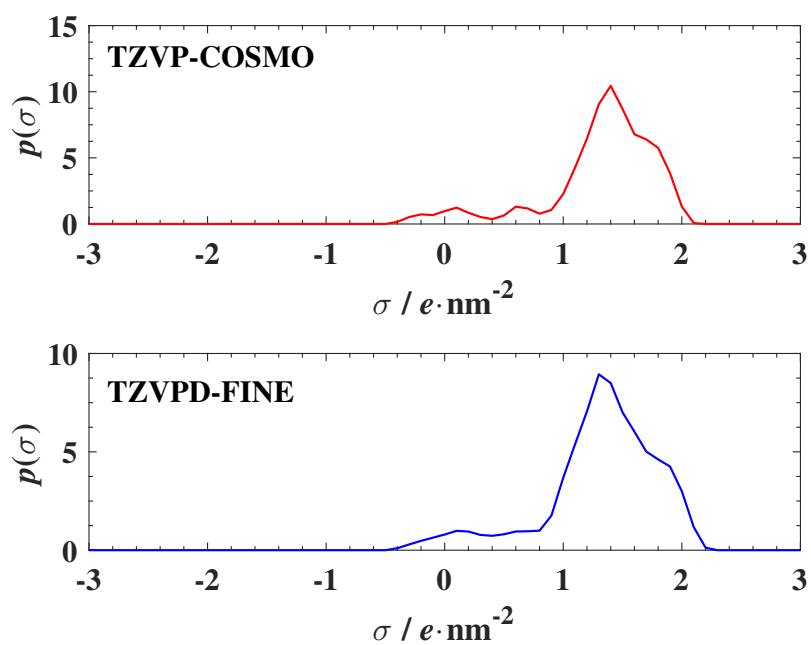
**Figure S140.**  $\sigma$ -profiles of SBF6 anion (abbreviations explained in the supplied Microsoft Excel spreadsheet, Table S1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



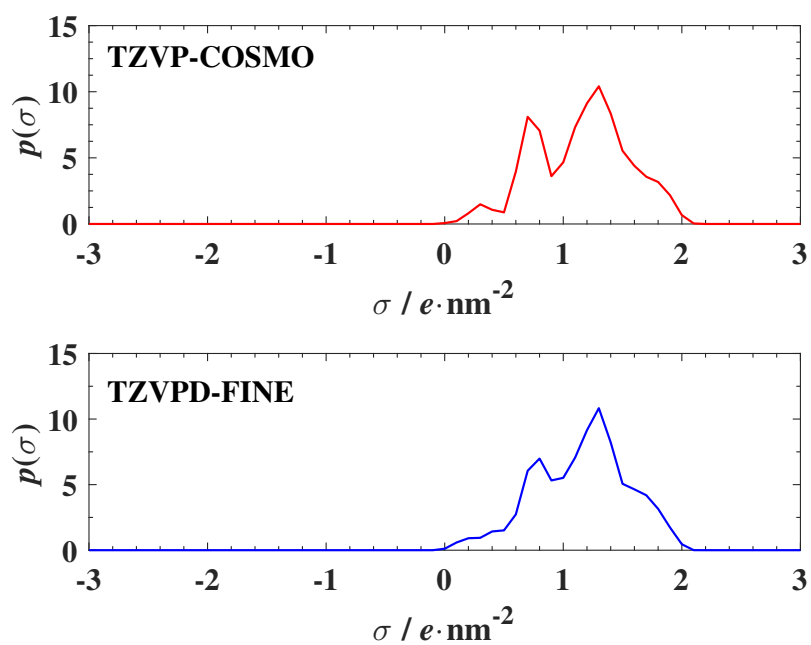
**Figure S141.**  $\sigma$ -profiles of CL anion (abbreviations explained in the supplied Microsoft Excel spreadsheet, Table S1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



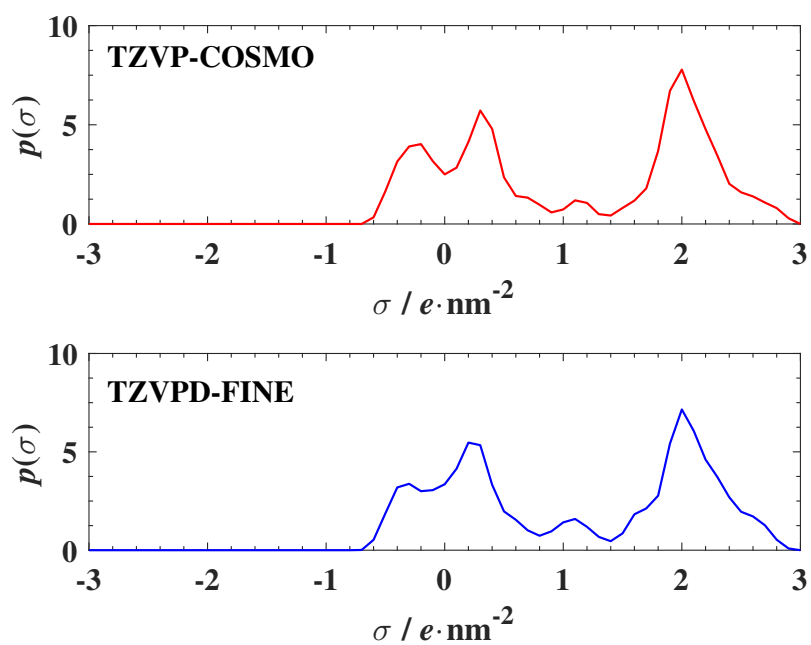
**Figure S142.**  $\sigma$ -profiles of BR anion (abbreviations explained in the supplied Microsoft Excel spreadsheet, Table S1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



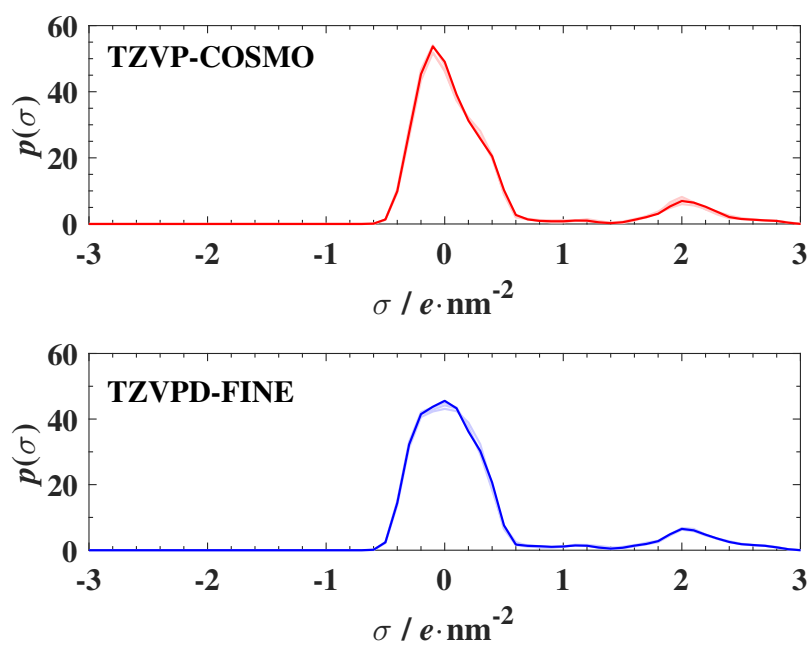
**Figure S143.**  $\sigma$ -profiles of  $\text{NO}_3$  anion (abbreviations explained in the supplied Microsoft Excel spreadsheet, Table S1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



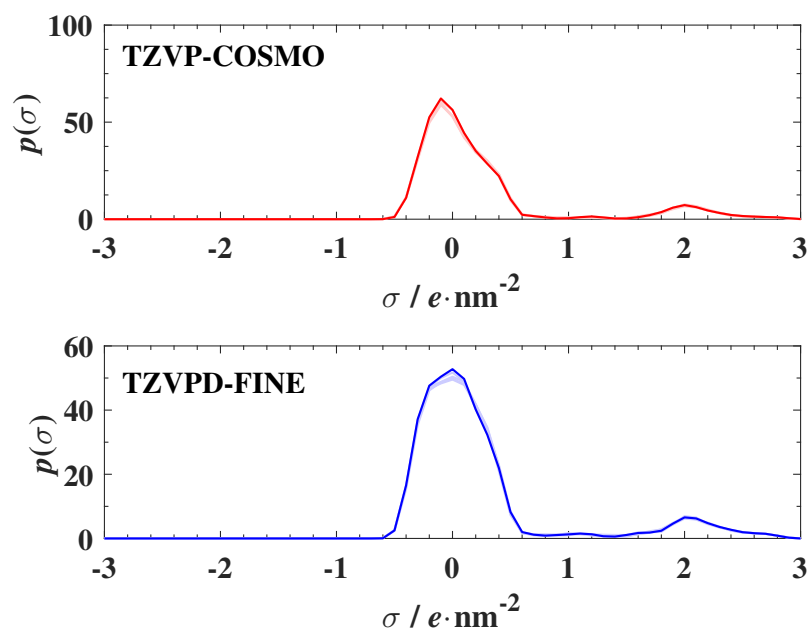
**Figure S144.**  $\sigma$ -profiles of SCN anion (abbreviations explained in the supplied Microsoft Excel spreadsheet, Table S1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



**Figure S145.**  $\sigma$ -profiles of AC anion (abbreviations explained in the supplied Microsoft Excel spreadsheet, Table S1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).

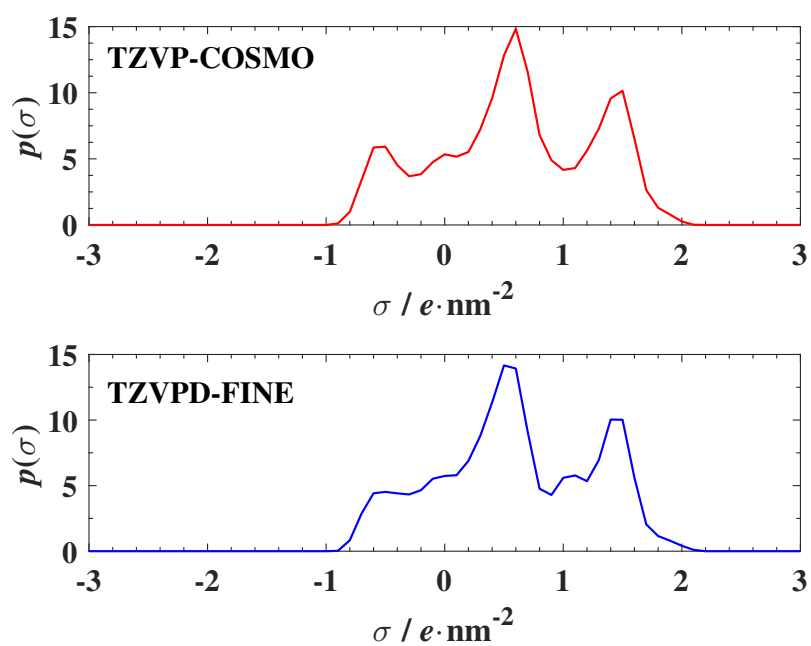


**Figure S146.**  $\sigma$ -profiles of 14AC anion (abbreviations explained in the supplied Microsoft Excel spreadsheet, Table S1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).

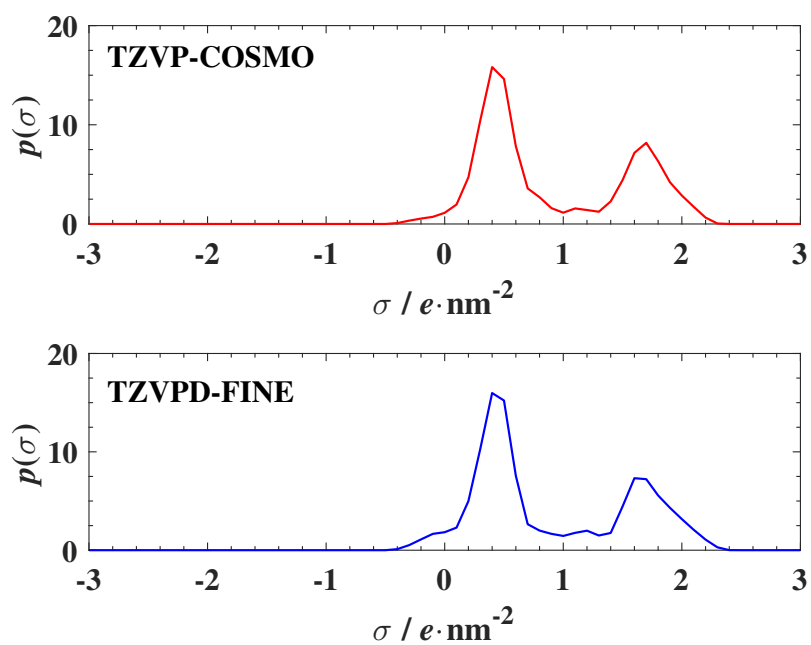


**Figure S147.**  $\sigma$ -profiles of 16AC anion (abbreviations explained in the supplied Microsoft Excel spreadsheet, Table S1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).

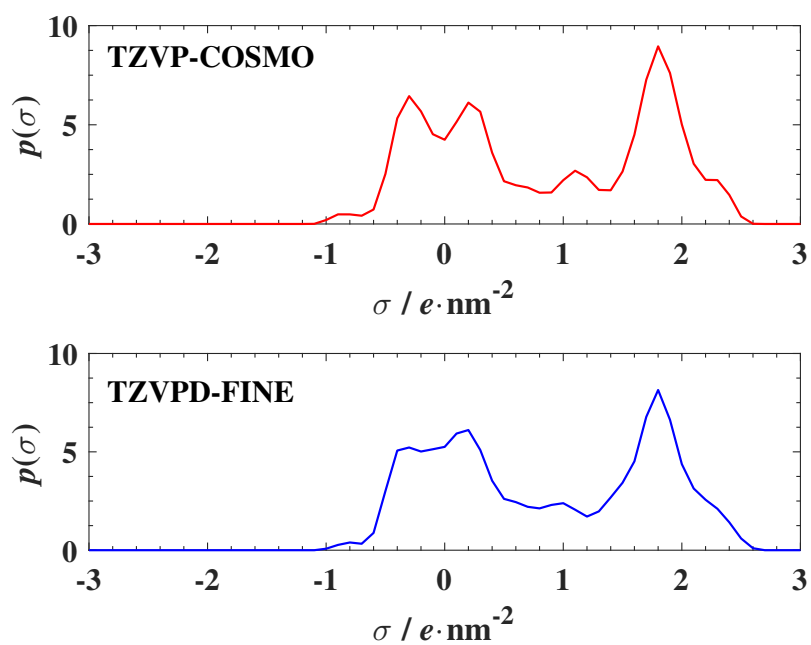




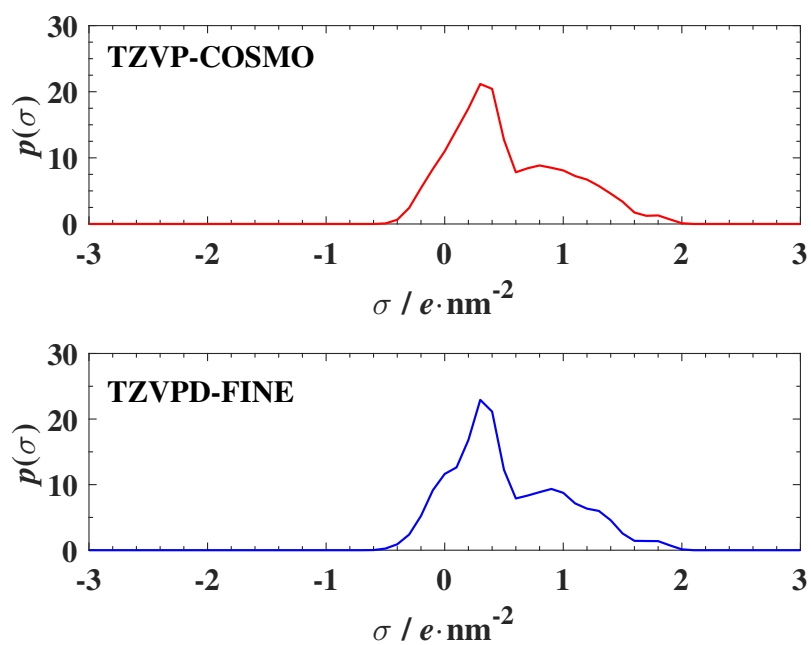
**Figure S148.**  $\sigma$ -profiles of PH-COO[1], SH[2] anion (abbreviations explained in the supplied Microsoft Excel spreadsheet, Table S1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



**Figure S149.**  $\sigma$ -profiles of TFA anion (abbreviations explained in the supplied Microsoft Excel spreadsheet, Table S1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



**Figure S150.**  $\sigma$ -profiles of LA anion (abbreviations explained in the supplied Microsoft Excel spreadsheet, Table S1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



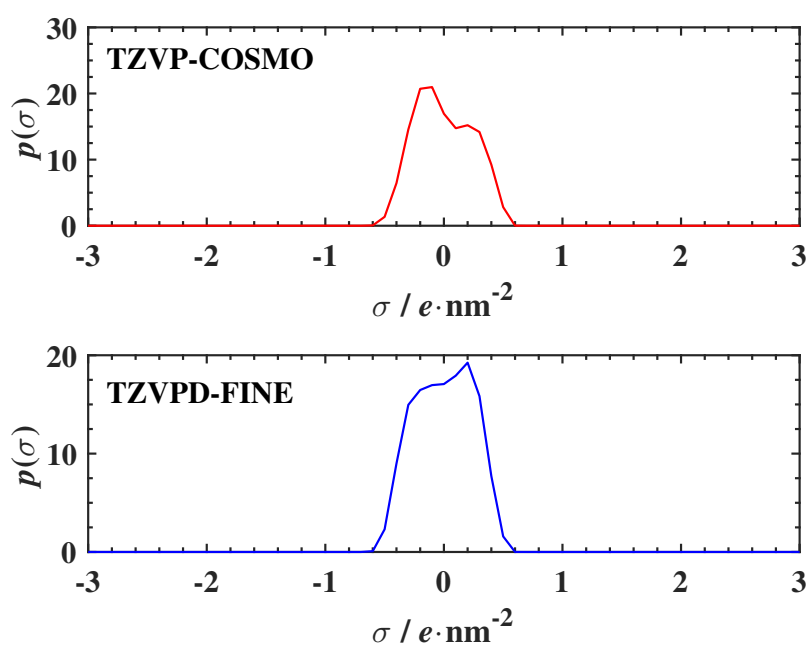
**Figure S151.**  $\sigma$ -profiles of TDI anion (abbreviations explained in the supplied Microsoft Excel spreadsheet, Table S1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).

### 3 $\sigma$ -Profiles of Solutes

S152 <i>n</i> -pentane . . . . .	160
S153 <i>n</i> -hexane . . . . .	161
S154 <i>n</i> -heptane . . . . .	162
S155 <i>n</i> -octane . . . . .	163
S156 <i>n</i> -nonane . . . . .	164
S157 <i>n</i> -decane . . . . .	165
S158 <i>n</i> -undecane . . . . .	166
S159 <i>n</i> -dodecane . . . . .	167
S160 <i>n</i> -tridecane . . . . .	168
S161 <i>n</i> -tetradecane . . . . .	169
S162 <i>n</i> -pentadecane . . . . .	170
S163 cyclopentane . . . . .	171
S164 cyclohexane . . . . .	172
S165 cycloheptane . . . . .	173
S166 cyclooctane . . . . .	174
S167 2,2-dimethylbutane . . . . .	175
S168 3-methylpentane . . . . .	176
S169 2,2,4-trimethylpentane . . . . .	177
S170 methylcyclopentane . . . . .	178
S171 methylcyclohexane . . . . .	179
S172 ethylcyclohexane . . . . .	180
S173 1-pentene . . . . .	181
S174 1-hexene . . . . .	182
S175 1-heptene . . . . .	183
S176 1-octene . . . . .	184
S177 1-nonene . . . . .	185
S178 1-decene . . . . .	186
S179 1-undecene . . . . .	187
S180 1-dodecene . . . . .	188
S181 cyclopentene . . . . .	189
S182 cyclohexene . . . . .	190
S183 1,3-cyclohexadiene . . . . .	191
S184 1-methylcyclohexene . . . . .	192
S185 1-pentyne . . . . .	193
S186 1-hexyne . . . . .	194
S187 1-heptyne . . . . .	195
S188 1-octyne . . . . .	196
S189 1-nonyne . . . . .	197
S190 1-decyne . . . . .	198
S191 benzene . . . . .	199
S192 toluene . . . . .	200
S193 ethylbenzene . . . . .	201
S194 <i>o</i> -xylene . . . . .	202
S195 <i>m</i> -xylene . . . . .	203
S196 <i>p</i> -xylene . . . . .	204
S197 <i>n</i> -propylbenzene . . . . .	205
S198 cumene . . . . .	206
S199 <i>n</i> -butylbenzene . . . . .	207
S200 <i>tert</i> -butylbenzene . . . . .	208
S201 <i>n</i> -pentylbenzene . . . . .	209
S202 1,3,5-trimethylbenzene . . . . .	210
S203 styrene . . . . .	211
S204 $\alpha$ -methylstyrene . . . . .	212
S205 methanol . . . . .	213
S206 ethanol . . . . .	214

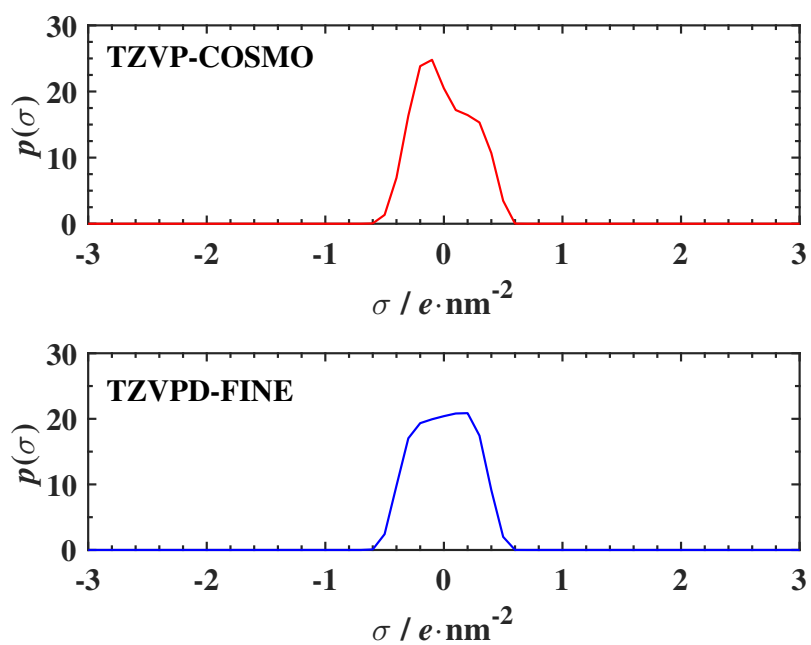
S207 1-propanol . . . . .	215
S208 2-propanol . . . . .	216
S209 1-butanol . . . . .	217
S210 2-butanol . . . . .	218
S211 2-methyl-1-propanol . . . . .	219
S212 <i>tert</i> -butanol . . . . .	220
S213 1-pentanol . . . . .	221
S214 1-hexanol . . . . .	222
S215 1-heptanol . . . . .	223
S216 2-pentanol . . . . .	224
S217 3-pentanol . . . . .	225
S218 3-methyl-1-butanol . . . . .	226
S219 2-methyl-2-butanol . . . . .	227
S220 cyclohexanol . . . . .	228
S221 2-methyl-2-pentanol . . . . .	229
S222 1,2-ethanediol . . . . .	230
S223 1,2-Propanediol . . . . .	231
S224 1,3-Propanediol . . . . .	232
S225 1,2-Butanediol . . . . .	233
S226 2,3-Butanediol . . . . .	234
S227 1,5-Pentanediol . . . . .	235
S228 methanal . . . . .	236
S229 ethanal . . . . .	237
S230 propanal . . . . .	238
S231 butanal . . . . .	239
S232 pentanal . . . . .	240
S233 hexanal . . . . .	241
S234 heptanal . . . . .	242
S235 octanal . . . . .	243
S236 acetone . . . . .	244
S237 butanone . . . . .	245
S238 2-pentanone . . . . .	246
S239 3-pentanone . . . . .	247
S240 2-hexanone . . . . .	248
S241 3-hexanone . . . . .	249
S242 cyclopentanone . . . . .	250
S243 cyclohexanone . . . . .	251
S244 diethyl ether . . . . .	252
S245 di- <i>n</i> -propyl ether . . . . .	253
S246 di- <i>iso</i> -propyl ether . . . . .	254
S247 di- <i>n</i> -butyl ether . . . . .	255
S248 <i>tert</i> -butylmethyl ether . . . . .	256
S249 <i>tert</i> -butylethyl ether . . . . .	257
S250 <i>tert</i> -amylmethyl ether . . . . .	258
S251 acetic acid . . . . .	259
S252 butyric acid . . . . .	260
S253 1,2-dimethoxyethane . . . . .	261
S254 1,2-epoxypropane . . . . .	262
S255 1,2-epoxybutane . . . . .	263
S256 tetrahydrofuran . . . . .	264
S257 1,4-dioxane . . . . .	265
S258 methyl acetate . . . . .	266
S259 ethyl acetate . . . . .	267
S260 butyl acetate . . . . .	268
S261 vinyl acetate . . . . .	269
S262 methyl propanoate . . . . .	270

S263 methyl butanoate . . . . .	271
S264 methyl pentanoate . . . . .	272
S265 methyl hexanoate . . . . .	273
S266 methyl heptanoate . . . . .	274
S267 dimethyl carbonate . . . . .	275
S268 acetonitrile . . . . .	276
S269 triethylamine . . . . .	277
S270 nitromethane . . . . .	278
S271 1-nitropropane . . . . .	279
S272 <i>N,N</i> -dimethylformamide . . . . .	280
S273 pyridine . . . . .	281
S274 dichloromethane . . . . .	282
S275 trichloromethane . . . . .	283
S276 tetrachloromethane . . . . .	284
S277 1,2-dichloroethane . . . . .	285
S278 trichloroethylene . . . . .	286
S279 2,2,2-trifluoroethanol . . . . .	287
S280 halothane . . . . .	288
S281 bromobenzene . . . . .	289
S282 chlorobenzene . . . . .	290
S283 thiophene . . . . .	291
S284 water . . . . .	292
S285 $\alpha$ -pinene . . . . .	293
S286 $\beta$ -pinene . . . . .	294
S287 (-)-borneol . . . . .	295
S288 (-)-isopulegol . . . . .	296
S289 (-)-menthone . . . . .	297
S290 (1 <i>R</i> )-(-)-fenchone . . . . .	298
S291 ( <i>R</i> )-(+)-camphor . . . . .	299
S292 ( <i>S</i> )-(+)-carvone . . . . .	300
S293 carvacrol . . . . .	301
S294 DL-citronellol . . . . .	302
S295 eucalyptol . . . . .	303
S296 eugenol . . . . .	304
S297 geraniol . . . . .	305
S298 L-(-)-menthol . . . . .	306
S299 linalool . . . . .	307
S300 thymol . . . . .	308
S301 $\alpha$ -pinene oxide . . . . .	309

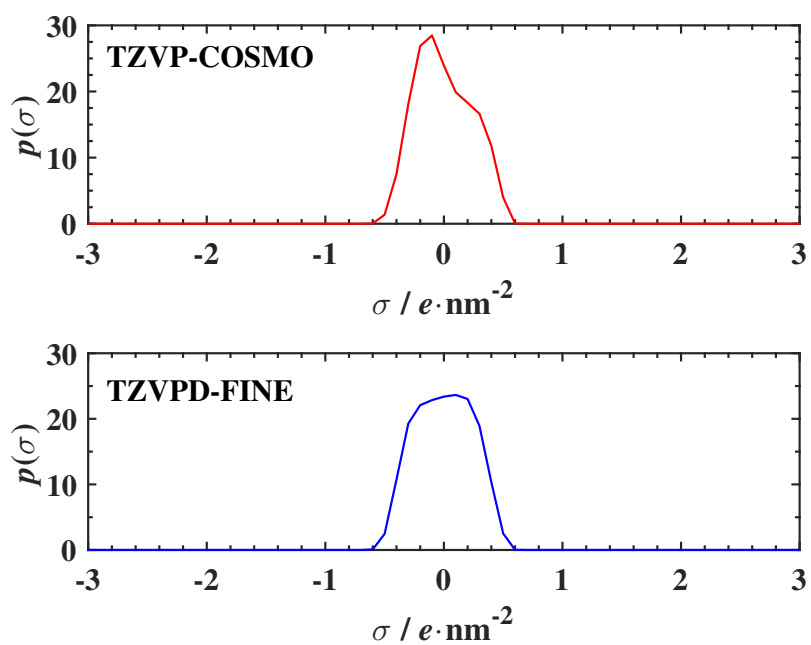


**Figure S152.**  $\sigma$ -profiles of *n*-pentane (CAS-RN: 109-66-0) obtained from screening charge distributions calculated at the BP-TZVP-COSMO level and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).

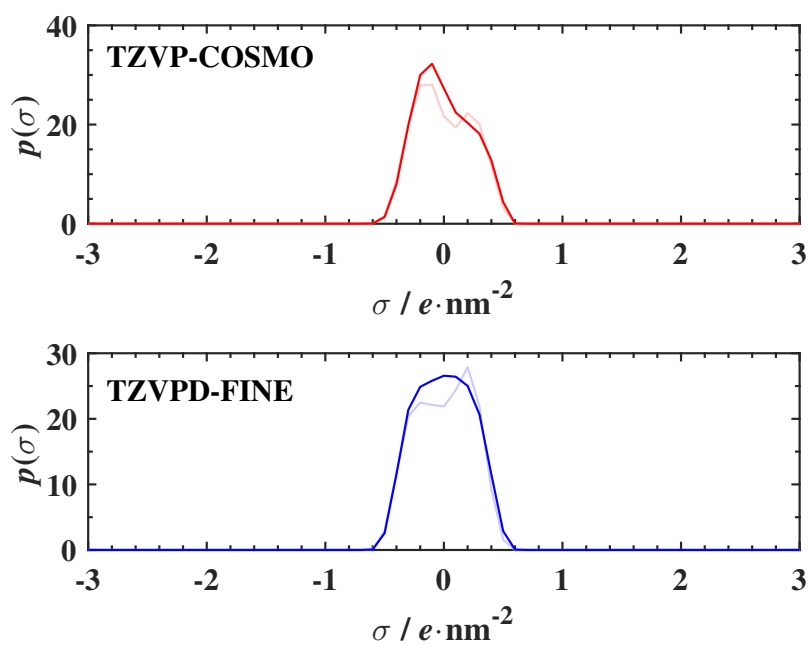




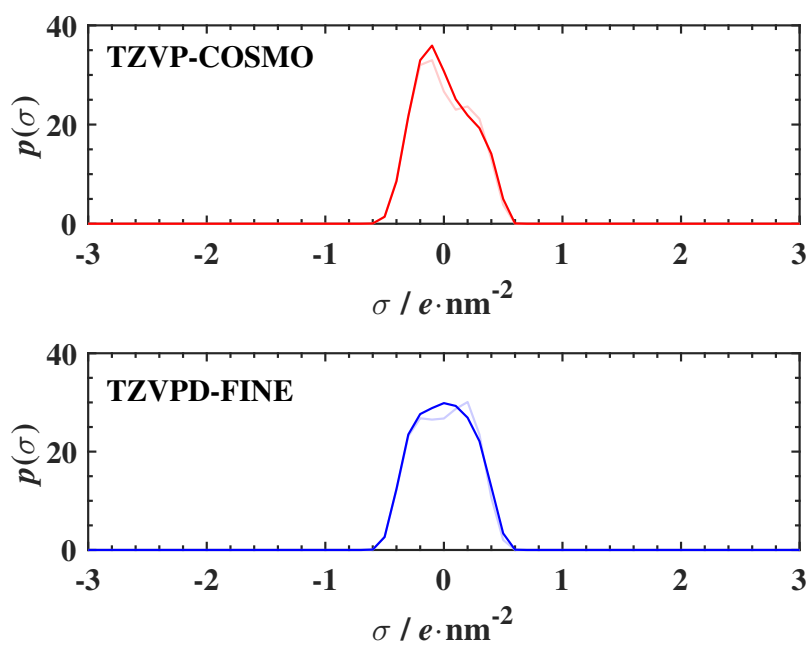
**Figure S153.**  $\sigma$ -profiles of *n*-hexane (CAS-RN: 110-54-3) obtained from screening charge distributions calculated at the BP-TZVP-COSMO level and BP-TZVPD-FINE levels. Thick lines are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



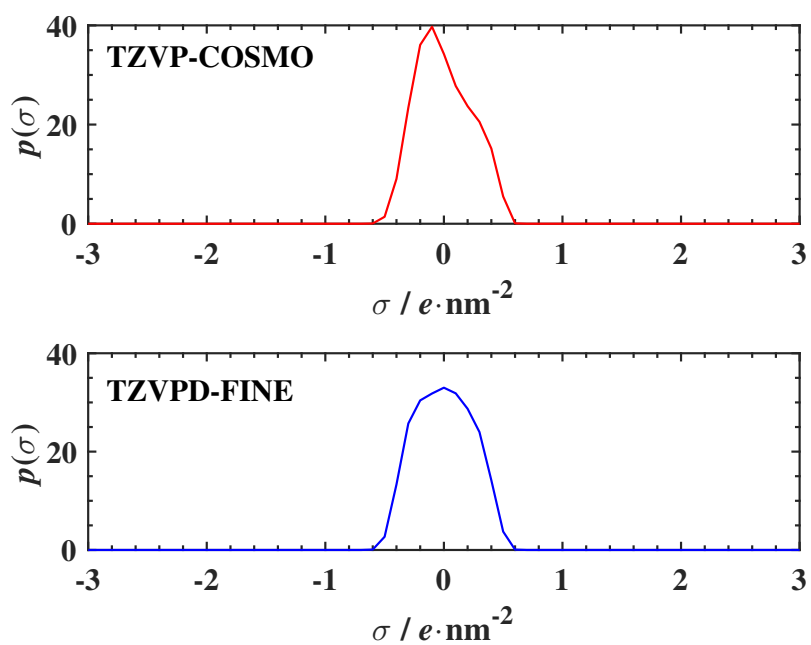
**Figure S154.**  $\sigma$ -profiles of *n*-heptane (CAS-RN: 142-82-5) obtained from screening charge distributions calculated at the BP-TZVP-COSMO level and BP-TZVPD-FINE levels. Thick lines are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



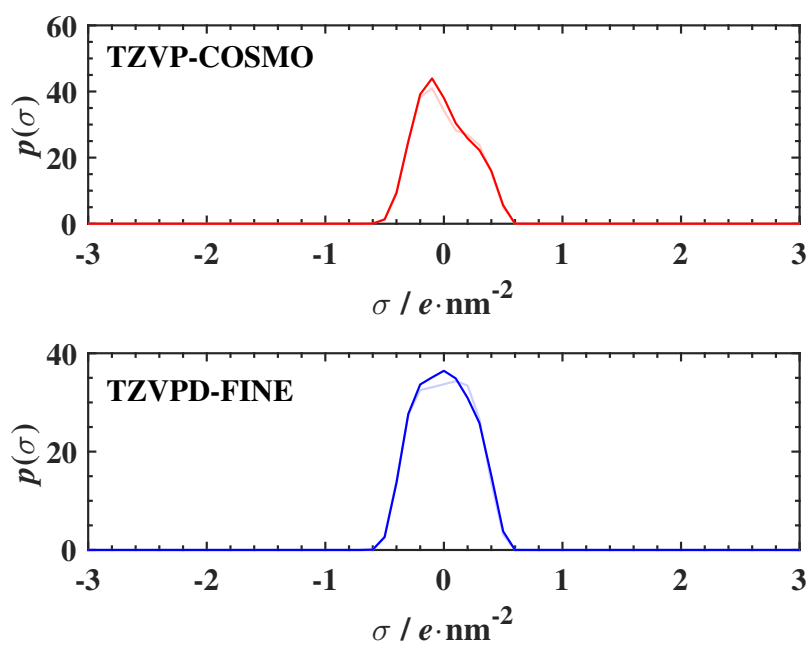
**Figure S155.**  $\sigma$ -profiles of *n*-octane (CAS-RN: 111-65-9) obtained from screening charge distributions calculated at the BP-TZVP-COSMO level and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



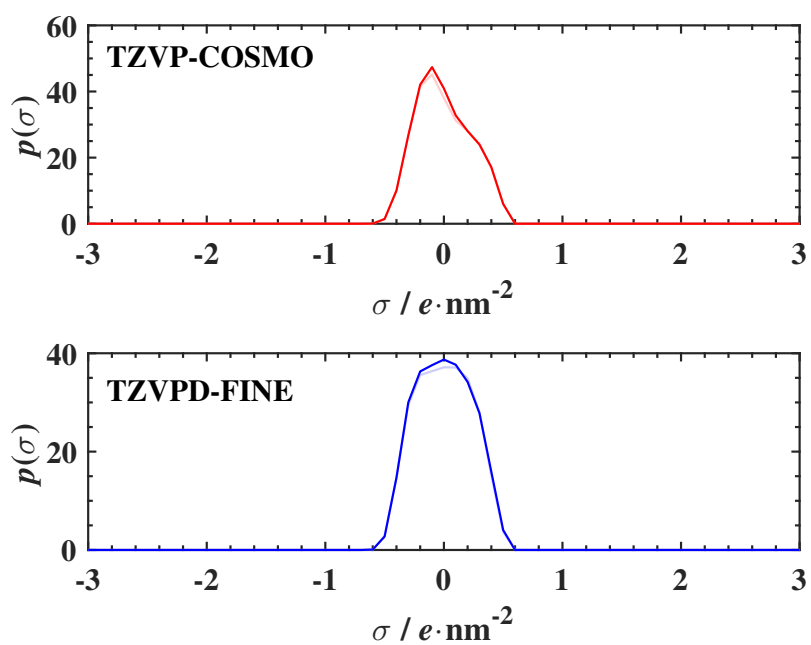
**Figure S156.**  $\sigma$ -profiles of *n*-nonane (CAS-RN: 111-84-2) obtained from screening charge distributions calculated at the BP-TZVP-COSMO level and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



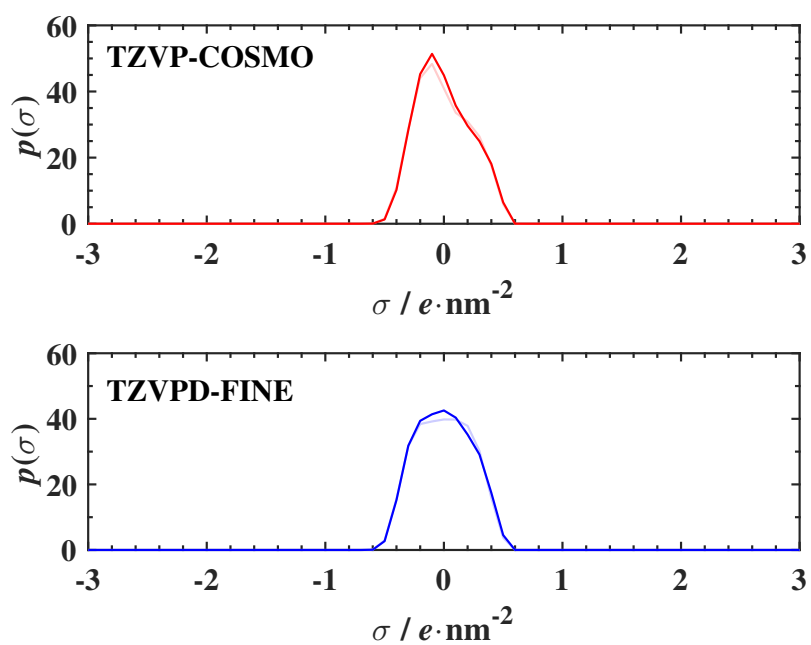
**Figure S157.**  $\sigma$ -profiles of *n*-decane (CAS-RN: 124-18-5) obtained from screening charge distributions calculated at the BP-TZVP-COSMO level and BP-TZVPD-FINE levels. Thick lines are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



**Figure S158.**  $\sigma$ -profiles of *n*-undecane (CAS-RN: 1120-21-4) obtained from screening charge distributions calculated at the BP-TZVP-COSMO level and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).

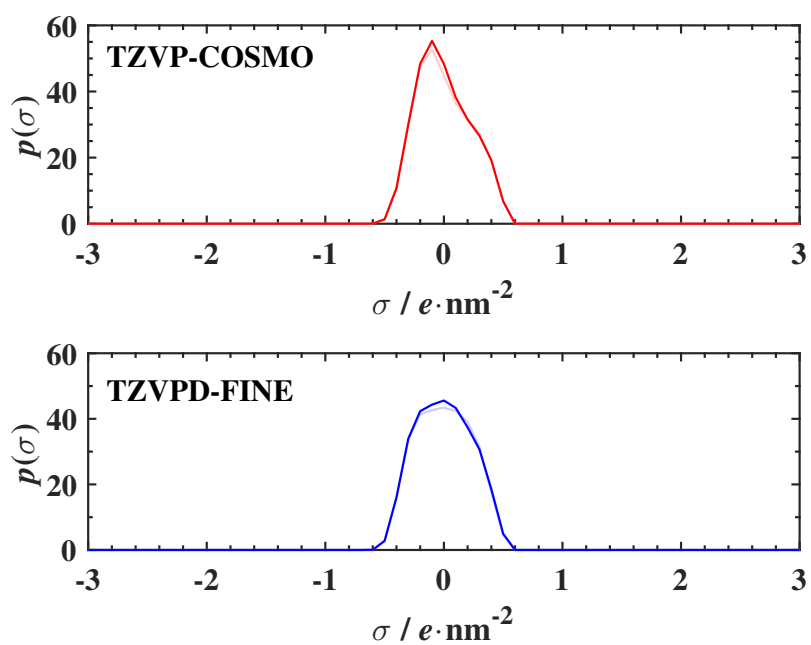


**Figure S159.**  $\sigma$ -profiles of *n*-dodecane (CAS-RN: 112-40-3) obtained from screening charge distributions calculated at the BP-TZVP-COSMO level and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).

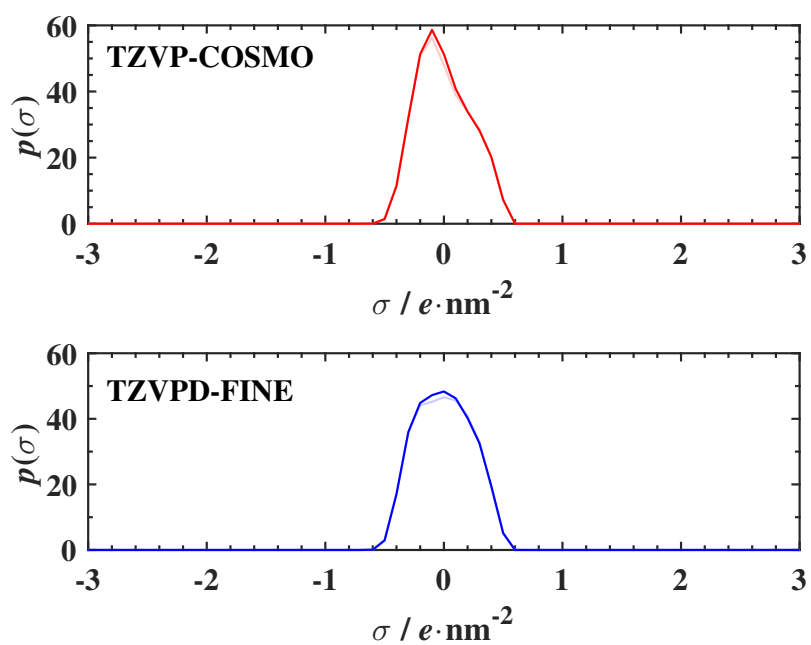


**Figure S160.**  $\sigma$ -profiles of *n*-tridecane (CAS-RN: 629-50-5) obtained from screening charge distributions calculated at the BP-TZVP-COSMO level and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).

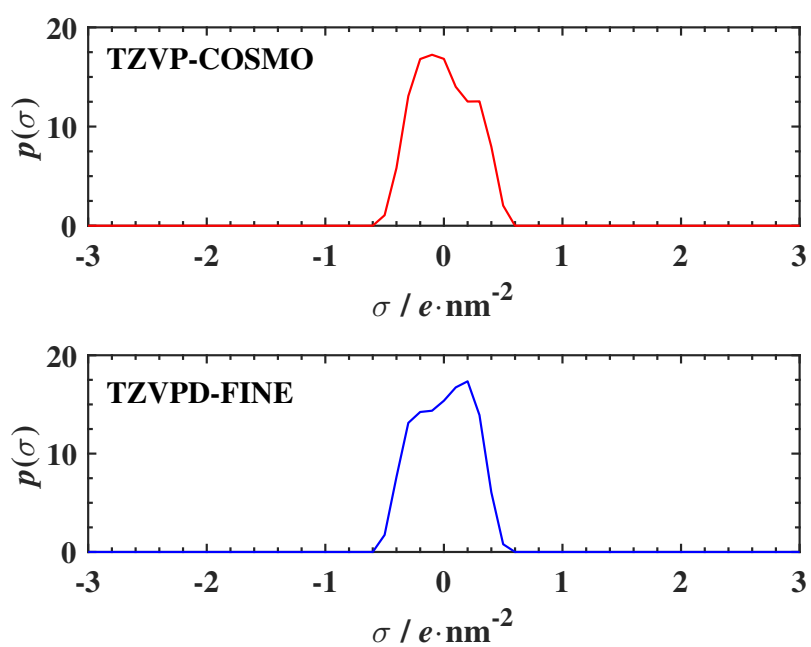




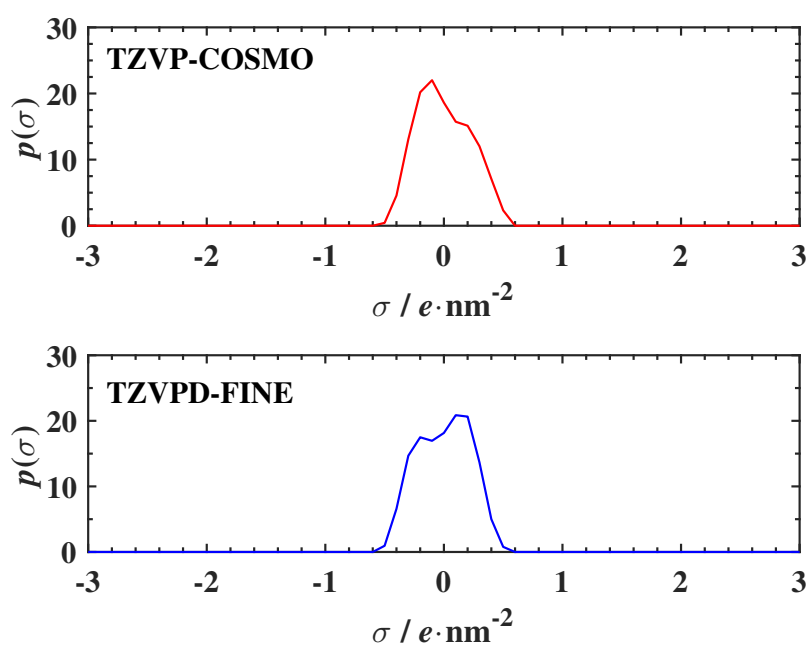
**Figure S161.**  $\sigma$ -profiles of *n*-tetradecane (CAS-RN: 629-59-4) obtained from screening charge distributions calculated at the BP-TZVP-COSMO level and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



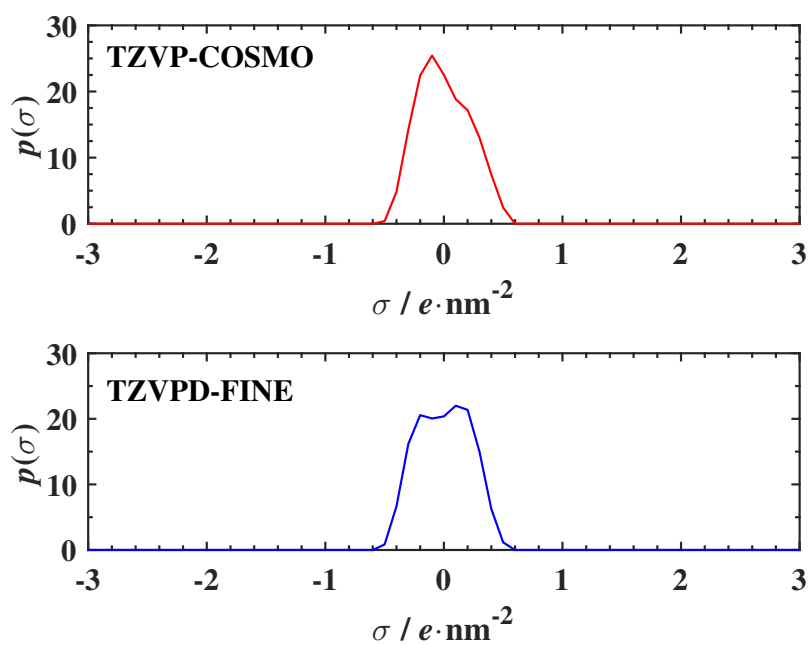
**Figure S162.**  $\sigma$ -profiles of *n*-pentadecane (CAS-RN: 629-62-9) obtained from screening charge distributions calculated at the BP-TZVP-COSMO level and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



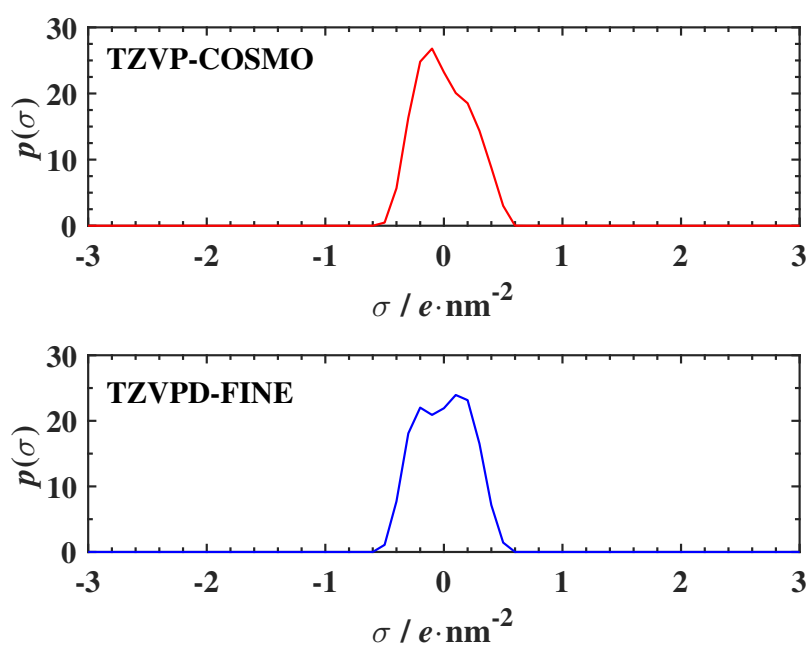
**Figure S163.**  $\sigma$ -profiles of cyclopentane (CAS-RN: 287-92-3) obtained from screening charge distributions calculated at the BP-TZVP-COSMO level and BP-TZVPD-FINE levels. Thick lines are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



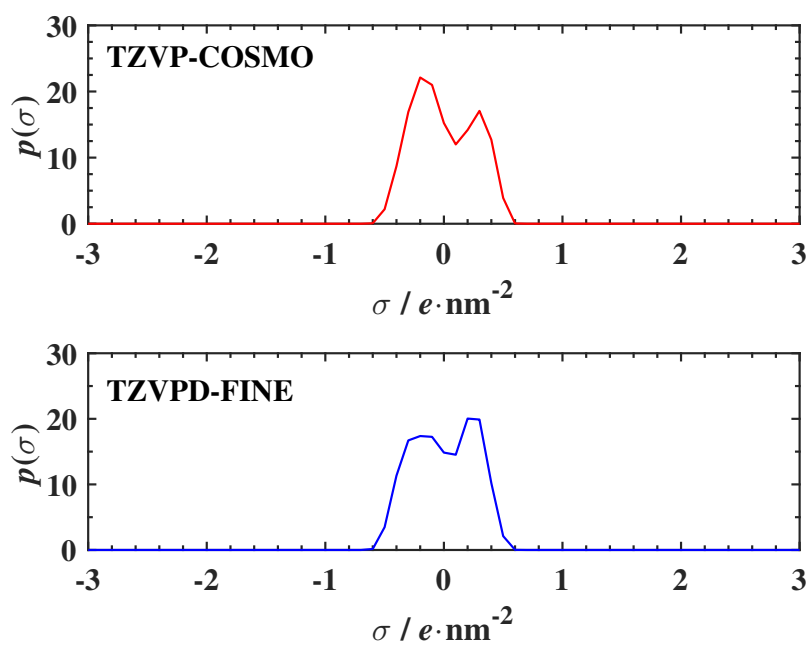
**Figure S164.**  $\sigma$ -profiles of cyclohexane (CAS-RN: 110-82-7) obtained from screening charge distributions calculated at the BP-TZVP-COSMO level and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



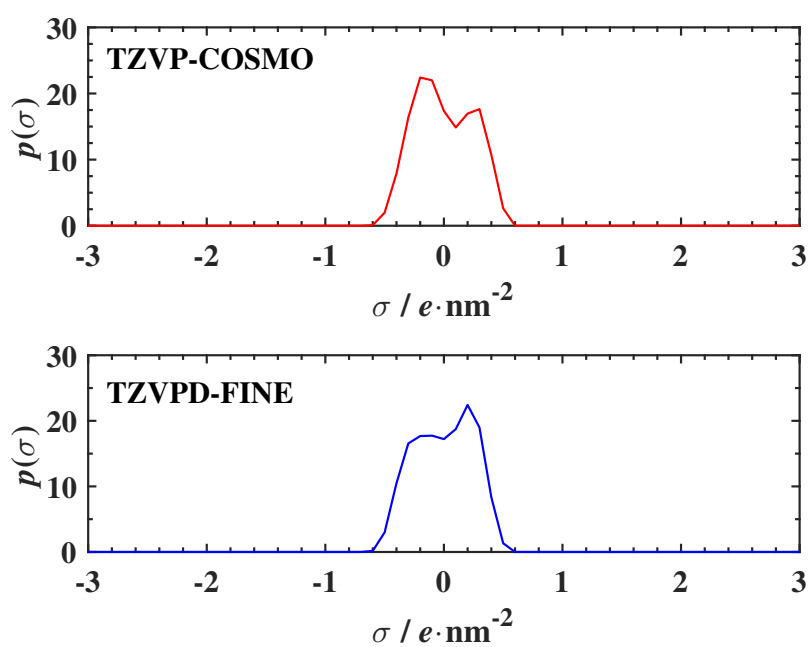
**Figure S165.**  $\sigma$ -profiles of cycloheptane (CAS-RN: 291-64-5) obtained from screening charge distributions calculated at the BP-TZVP-COSMO level and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



**Figure S166.**  $\sigma$ -profiles of cyclooctane (CAS-RN: 292-64-8) obtained from screening charge distributions calculated at the BP-TZVP-COSMO level and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).

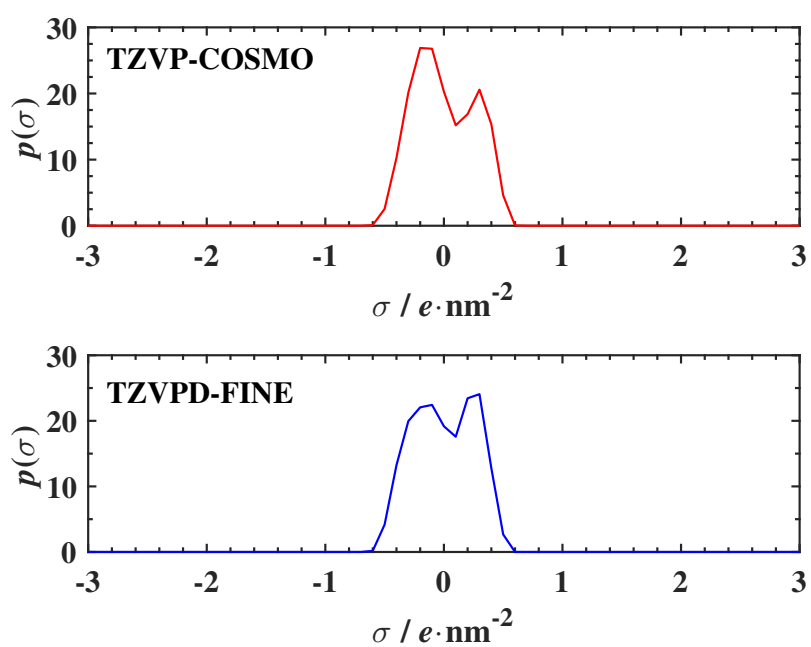


**Figure S167.**  $\sigma$ -profiles of 2,2-dimethylbutane (CAS-RN: 75-83-2) obtained from screening charge distributions calculated at the BP-TZVP-COSMO level and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).

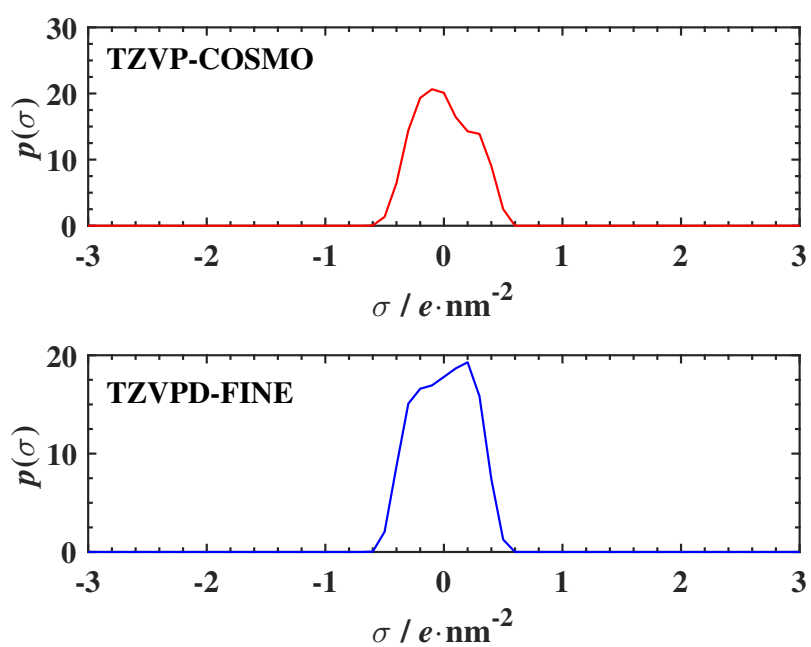


**Figure S168.**  $\sigma$ -profiles of 3-methylpentane (CAS-RN: 96-14-0) obtained from screening charge distributions calculated at the BP-TZVP-COSMO level and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).

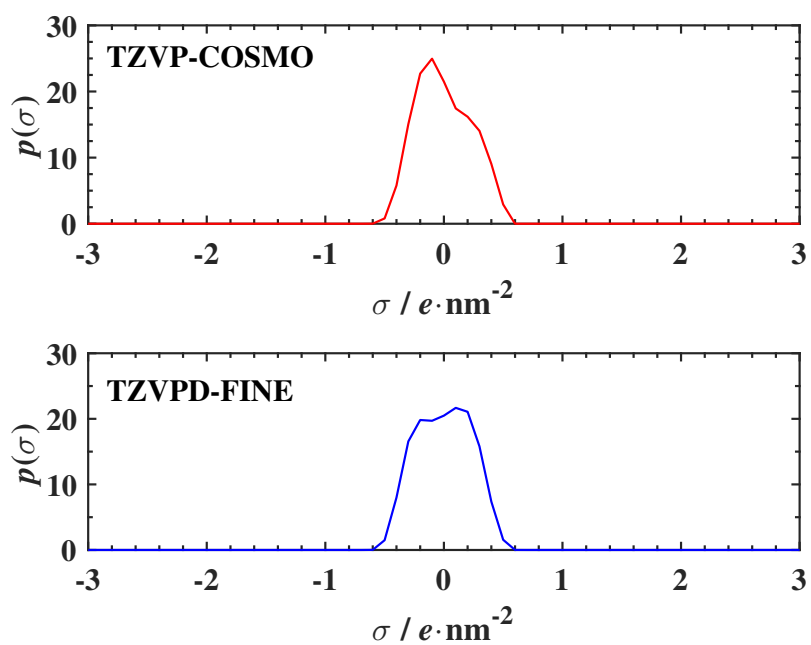




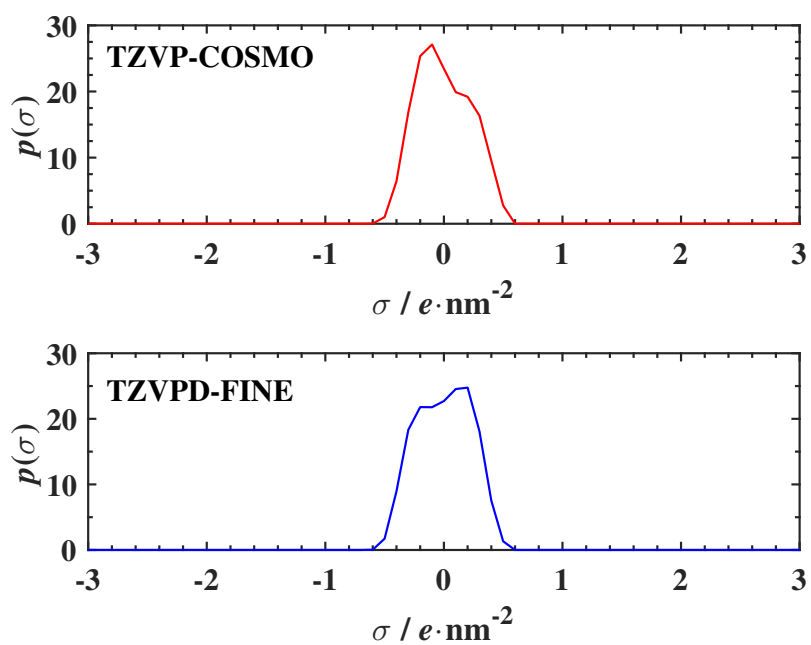
**Figure S169.**  $\sigma$ -profiles of 2,2,4-trimethylpentane (CAS-RN: 540-84-1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO level and BP-TZVPD-FINE levels. Thick lines are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



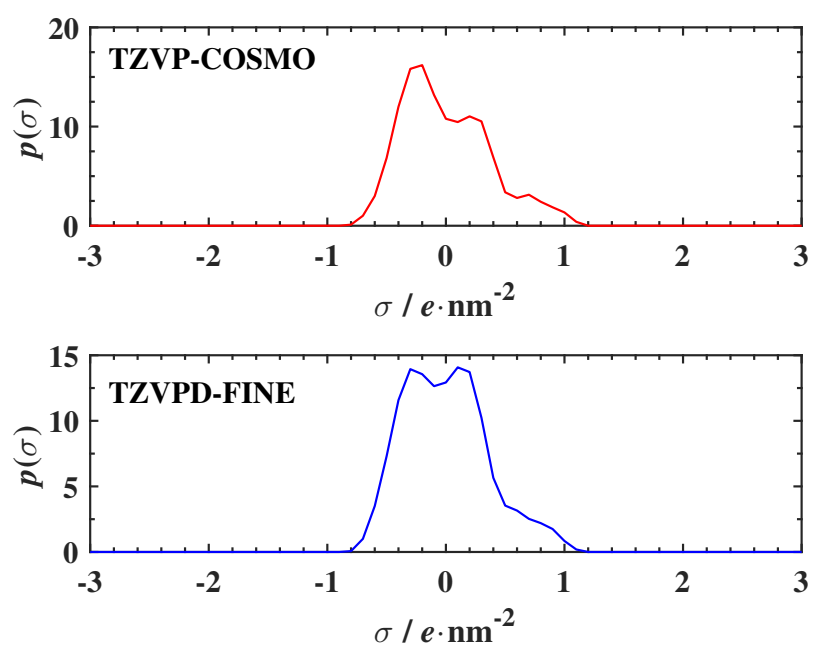
**Figure S170.**  $\sigma$ -profiles of methylcyclopentane (CAS-RN: 96-37-7) obtained from screening charge distributions calculated at the BP-TZVP-COSMO level and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



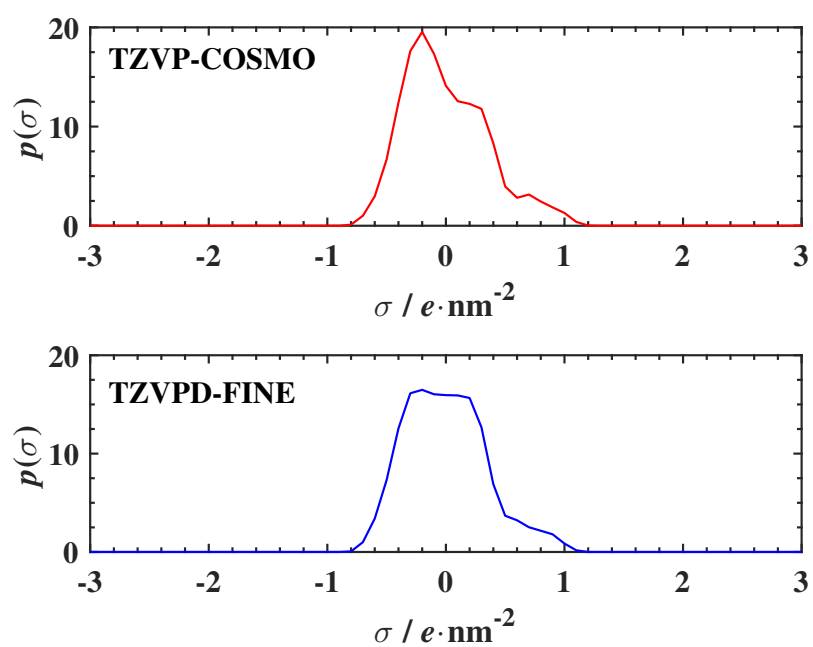
**Figure S171.**  $\sigma$ -profiles of methylcyclohexane (CAS-RN: 108-87-2) obtained from screening charge distributions calculated at the BP-TZVP-COSMO level and BP-TZVPD-FINE levels. Thick lines are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



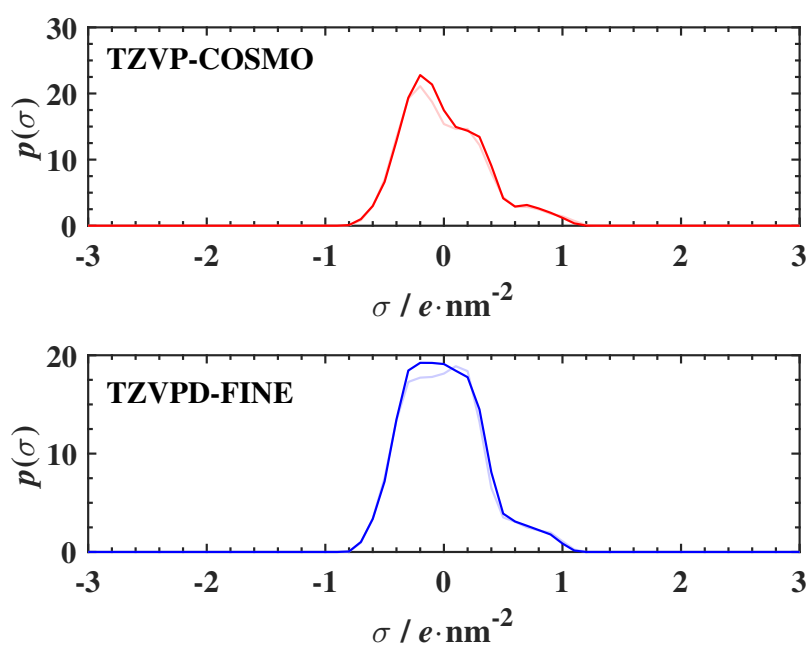
**Figure S172.**  $\sigma$ -profiles of ethylcyclohexane (CAS-RN: 1678-91-7) obtained from screening charge distributions calculated at the BP-TZVP-COSMO level and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



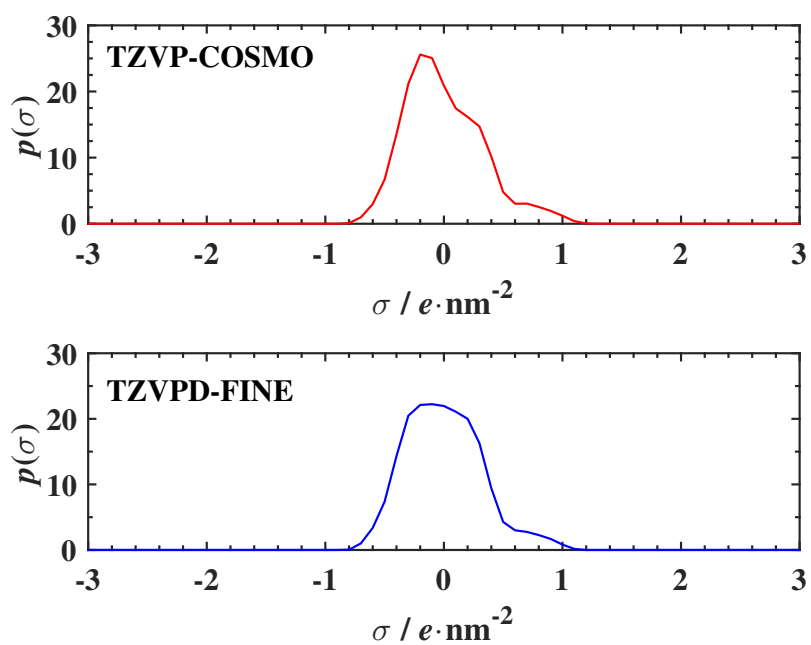
**Figure S173.**  $\sigma$ -profiles of 1-pentene (CAS-RN: 109-67-1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO level and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



**Figure S174.**  $\sigma$ -profiles of 1-hexene (CAS-RN: 592-41-6) obtained from screening charge distributions calculated at the BP-TZVP-COSMO level and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).

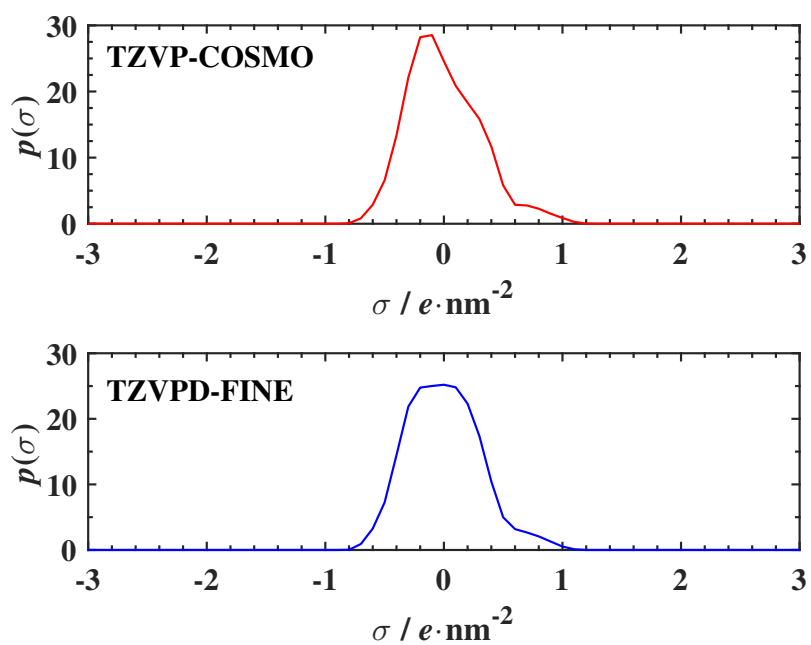


**Figure S175.**  $\sigma$ -profiles of 1-heptene (CAS-RN: 592-76-7) obtained from screening charge distributions calculated at the BP-TZVP-COSMO level and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).

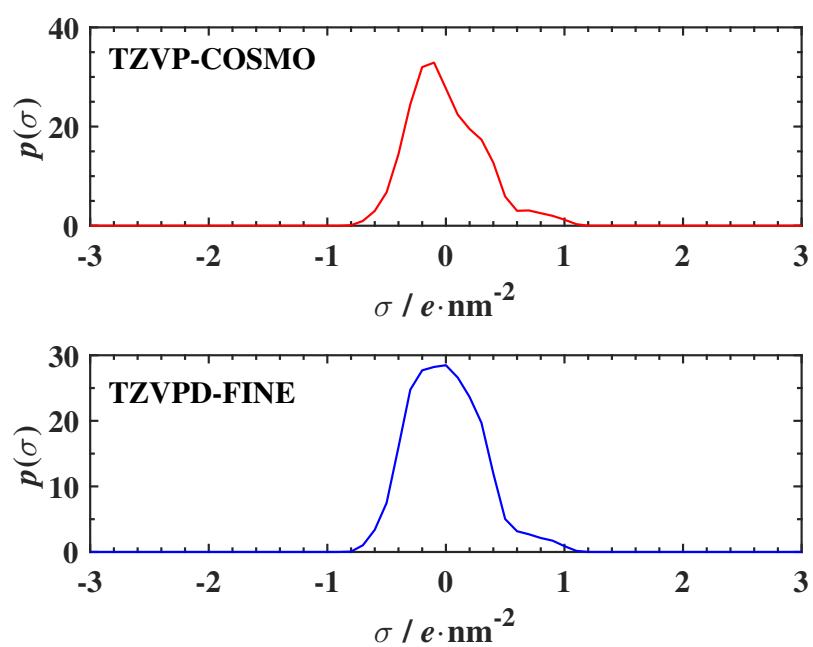


**Figure S176.**  $\sigma$ -profiles of 1-octene (CAS-RN: 111-66-0) obtained from screening charge distributions calculated at the BP-TZVP-COSMO level and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).

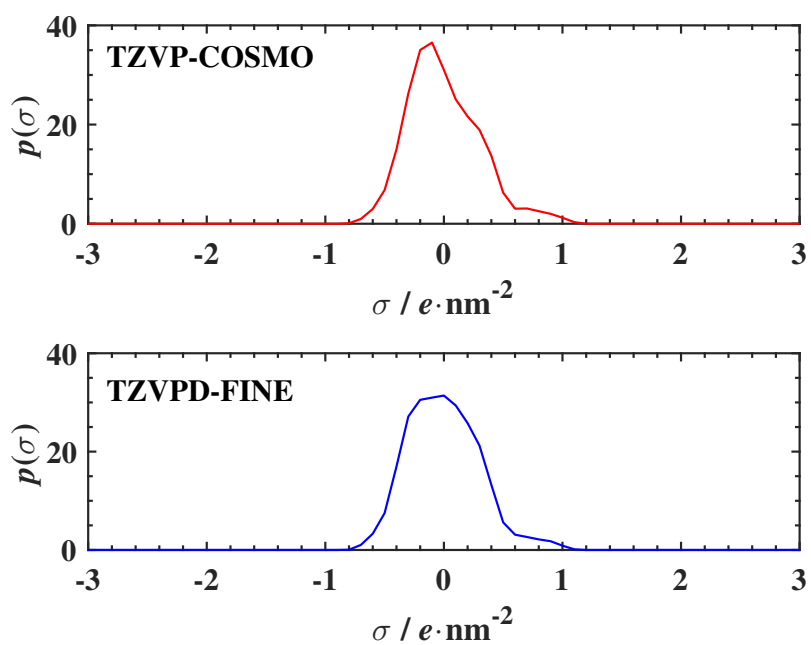




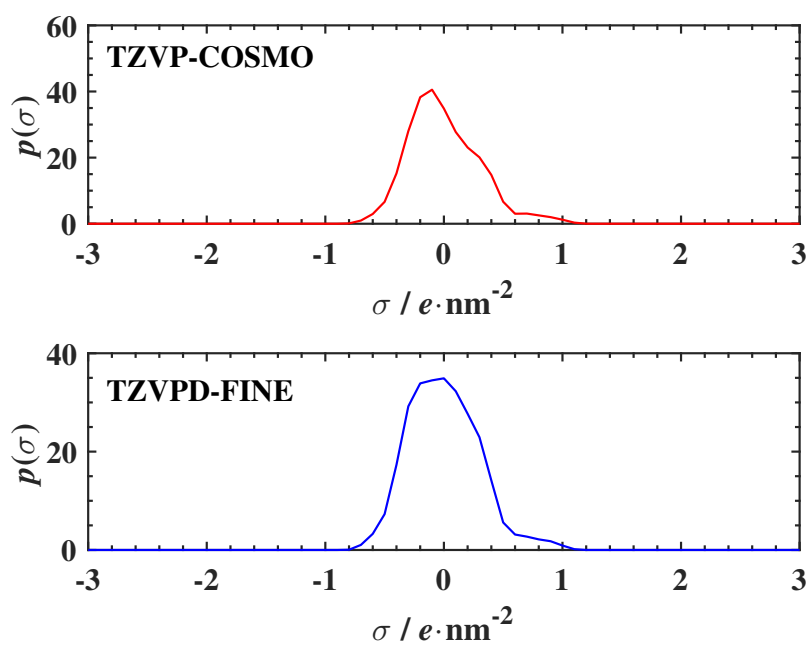
**Figure S177.**  $\sigma$ -profiles of 1-nonene (CAS-RN: 124-11-8) obtained from screening charge distributions calculated at the BP-TZVP-COSMO level and BP-TZVPD-FINE levels. Thick lines are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



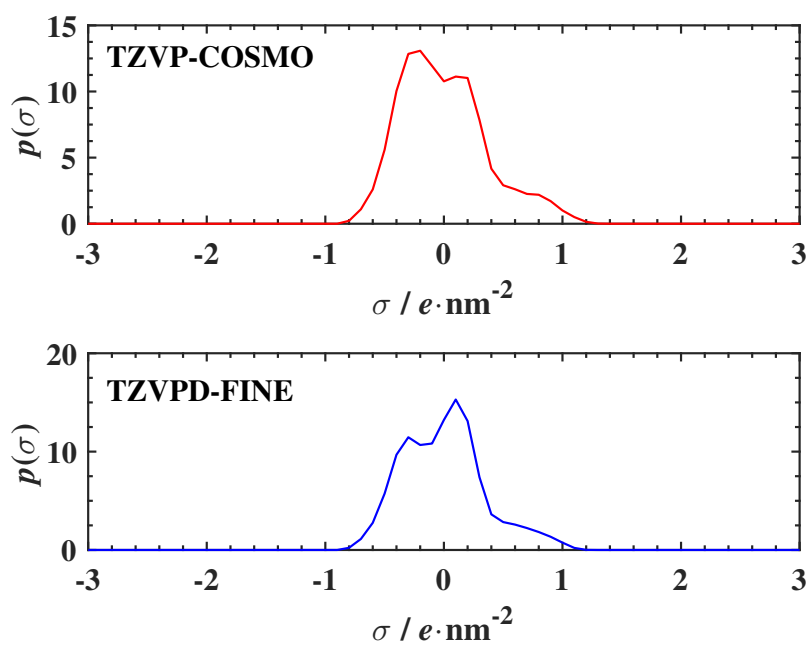
**Figure S178.**  $\sigma$ -profiles of 1-decene (CAS-RN: 872-5-9) obtained from screening charge distributions calculated at the BP-TZVP-COSMO level and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



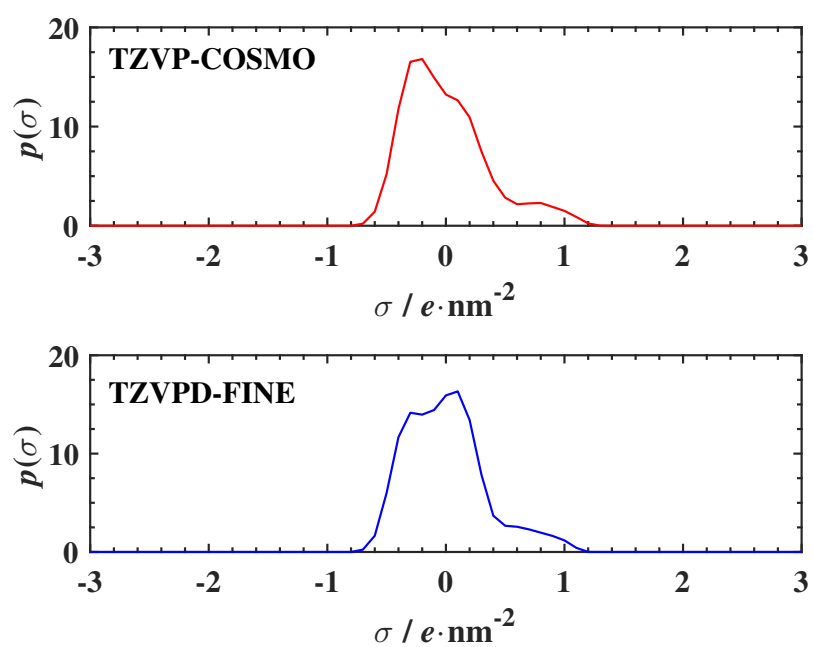
**Figure S179.**  $\sigma$ -profiles of 1-undecene (CAS-RN: 821-95-4) obtained from screening charge distributions calculated at the BP-TZVP-COSMO level and BP-TZVPD-FINE levels. Thick lines are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



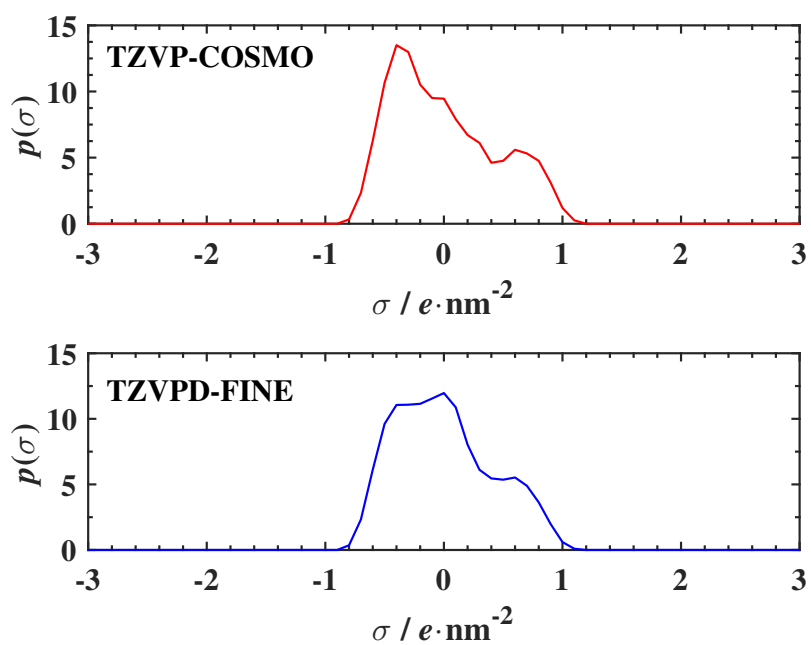
**Figure S180.**  $\sigma$ -profiles of 1-dodecene (CAS-RN: 112-41-4) obtained from screening charge distributions calculated at the BP-TZVP-COSMO level and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



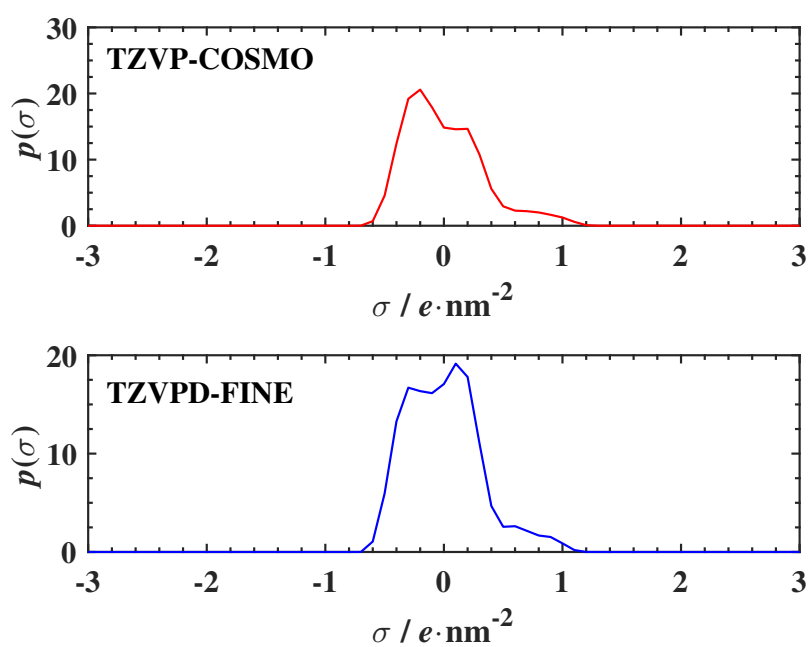
**Figure S181.**  $\sigma$ -profiles of cyclopentene (CAS-RN: 142-29-0) obtained from screening charge distributions calculated at the BP-TZVP-COSMO level and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



**Figure S182.**  $\sigma$ -profiles of cyclohexene (CAS-RN: 110-83-8) obtained from screening charge distributions calculated at the BP-TZVP-COSMO level and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).

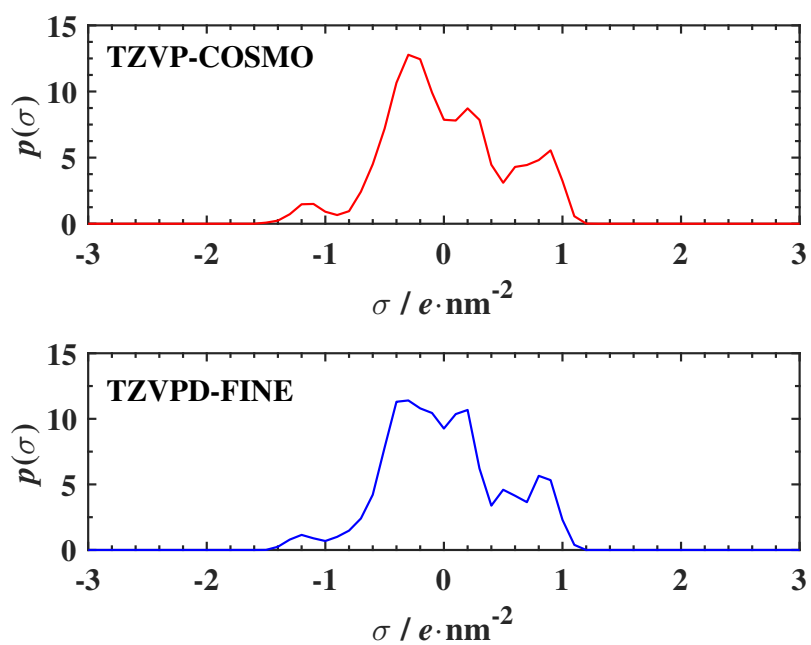


**Figure S183.**  $\sigma$ -profiles of 1,3-cyclohexadiene (CAS-RN: 592-57-4) obtained from screening charge distributions calculated at the BP-TZVP-COSMO level and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).

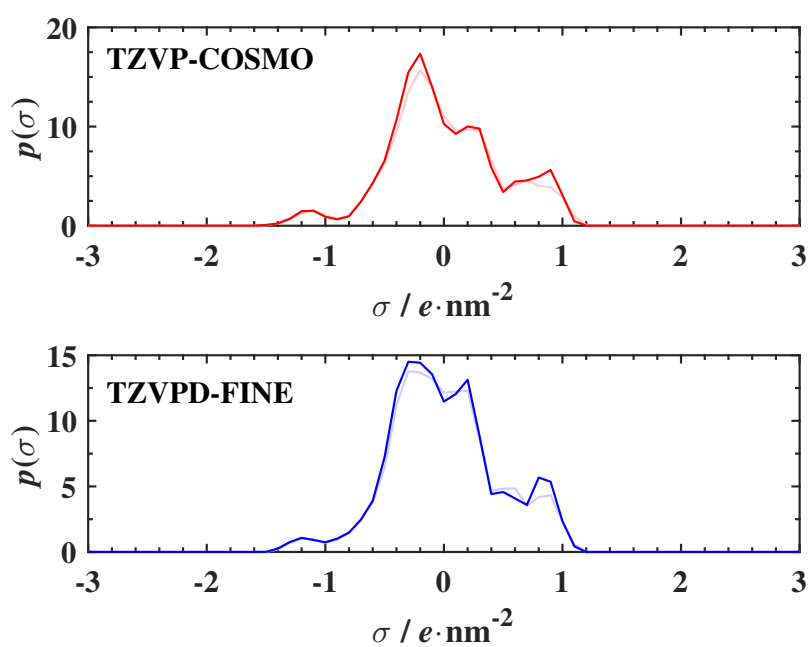


**Figure S184.**  $\sigma$ -profiles of 1-methylcyclohexene (CAS-RN: 591-49-1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO level and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).

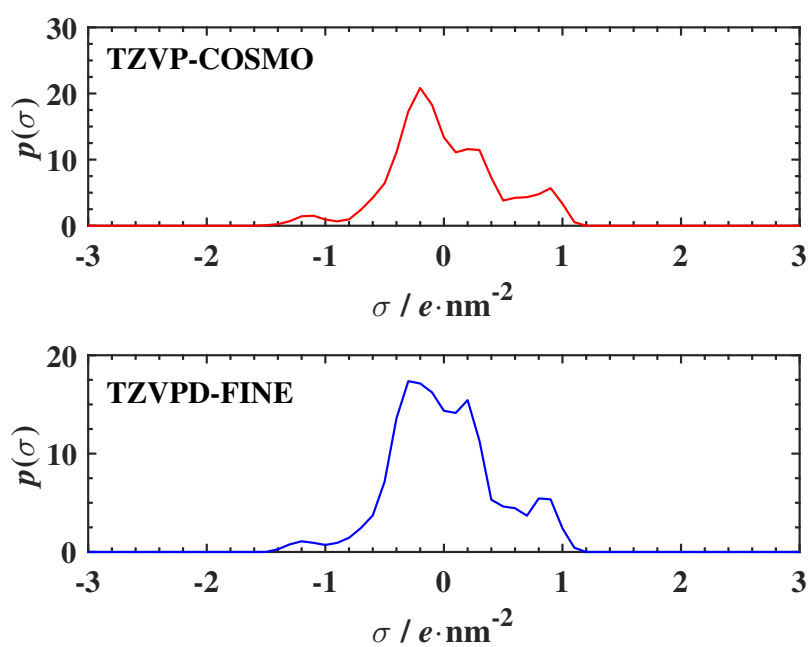




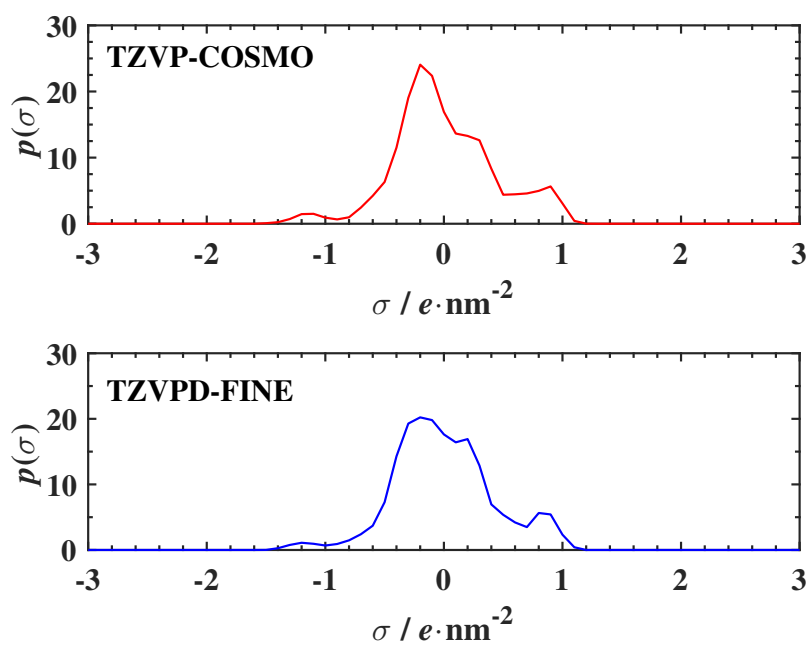
**Figure S185.**  $\sigma$ -profiles of 1-pentyne (CAS-RN: 627-19-0) obtained from screening charge distributions calculated at the BP-TZVP-COSMO level and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



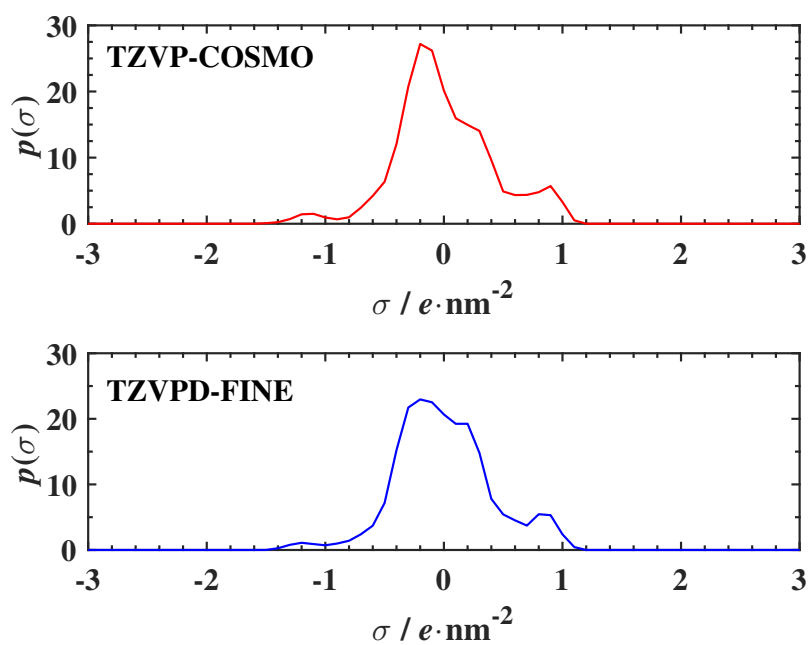
**Figure S186.**  $\sigma$ -profiles of 1-hexyne (CAS-RN: 693-2-7) obtained from screening charge distributions calculated at the BP-TZVP-COSMO level and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



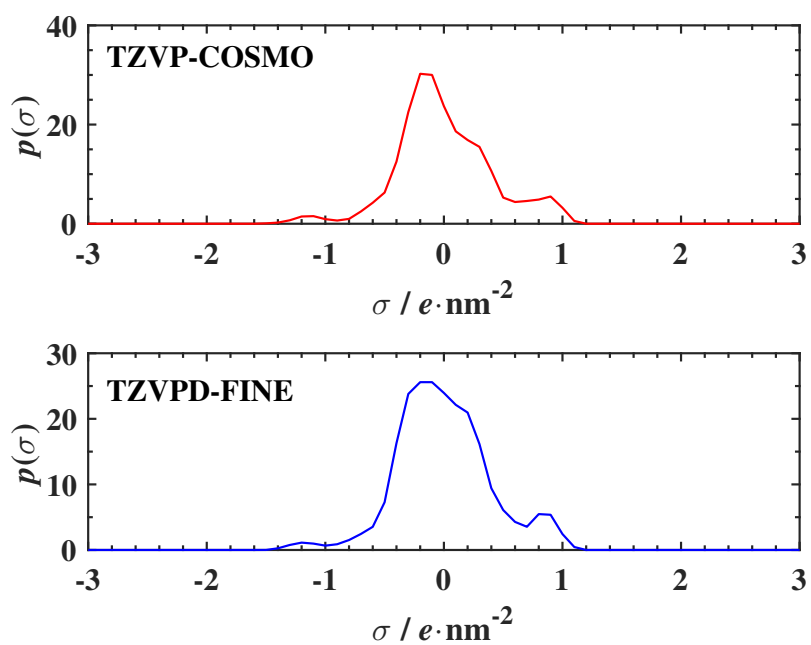
**Figure S187.**  $\sigma$ -profiles of 1-heptyne (CAS-RN: 628-71-7) obtained from screening charge distributions calculated at the BP-TZVP-COSMO level and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



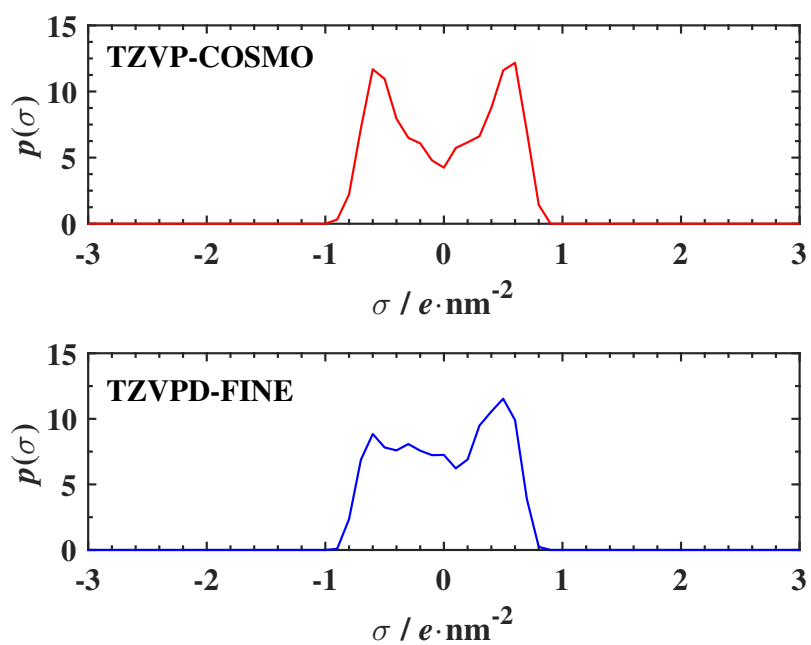
**Figure S188.**  $\sigma$ -profiles of 1-octyne (CAS-RN: 629-5-0) obtained from screening charge distributions calculated at the BP-TZVP-COSMO level and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



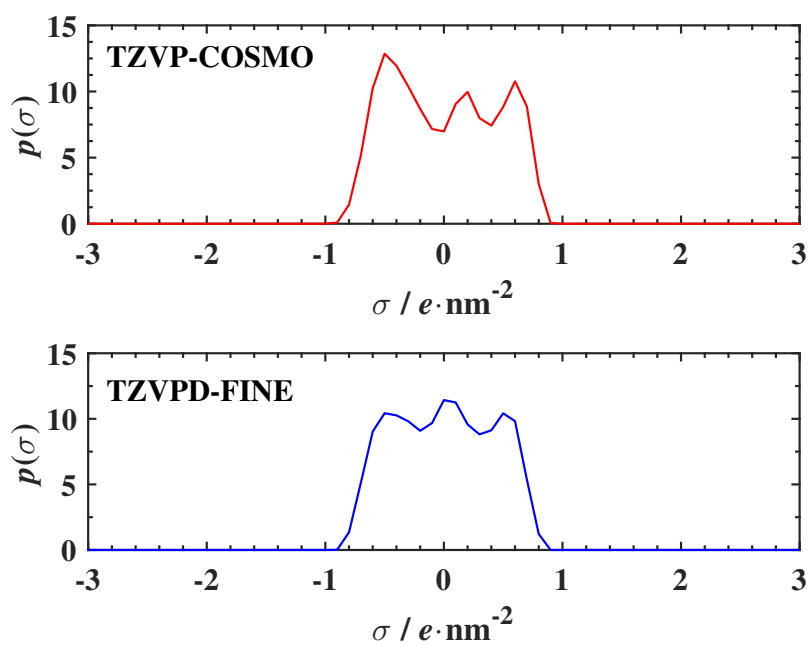
**Figure S189.**  $\sigma$ -profiles of 1-nonyne (CAS-RN: 3452-9-3) obtained from screening charge distributions calculated at the BP-TZVP-COSMO level and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



**Figure S190.**  $\sigma$ -profiles of 1-decyne (CAS-RN: 764-93-2) obtained from screening charge distributions calculated at the BP-TZVP-COSMO level and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).

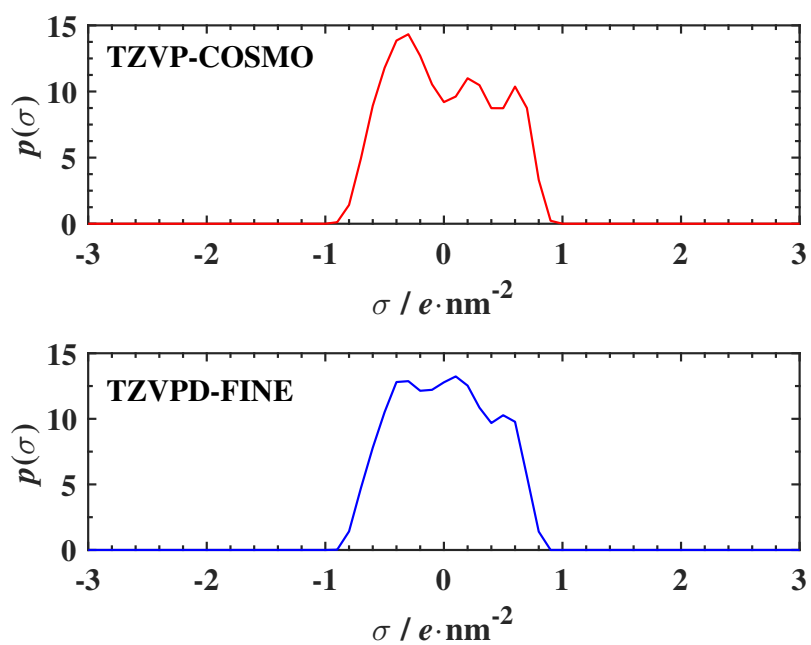


**Figure S191.**  $\sigma$ -profiles of benzene (CAS-RN: 71-43-2) obtained from screening charge distributions calculated at the BP-TZVP-COSMO level and BP-TZVPD-FINE levels. Thick lines are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).

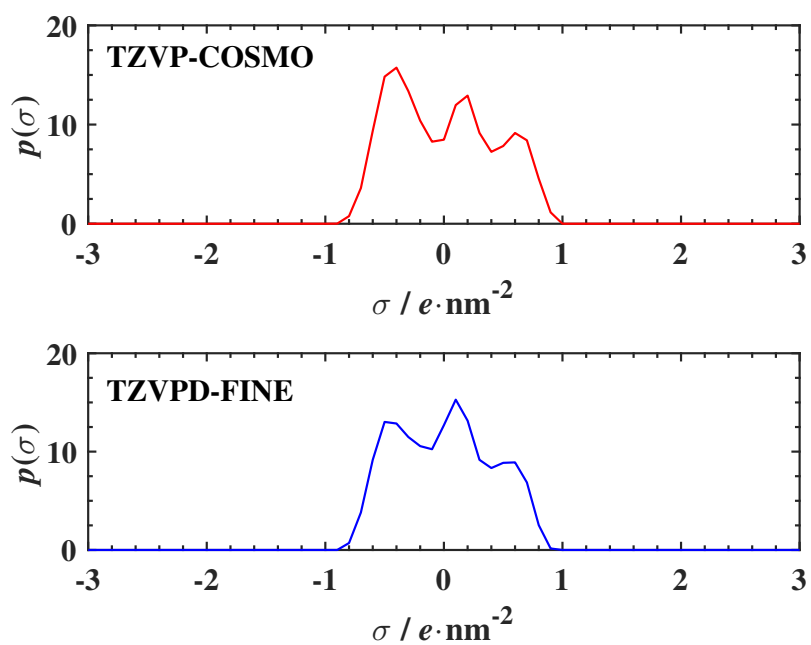


**Figure S192.**  $\sigma$ -profiles of toluene (CAS-RN: 108-88-3) obtained from screening charge distributions calculated at the BP-TZVP-COSMO level and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).

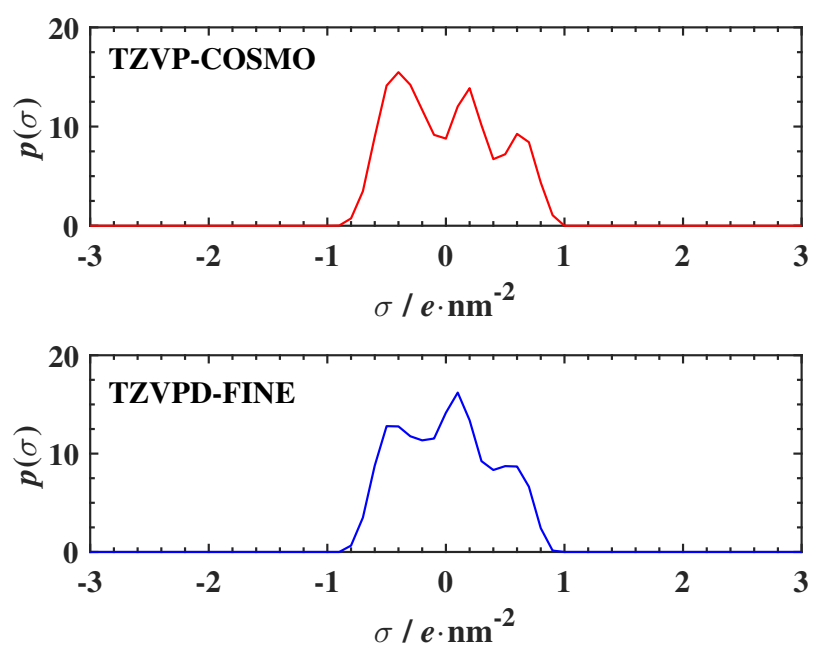




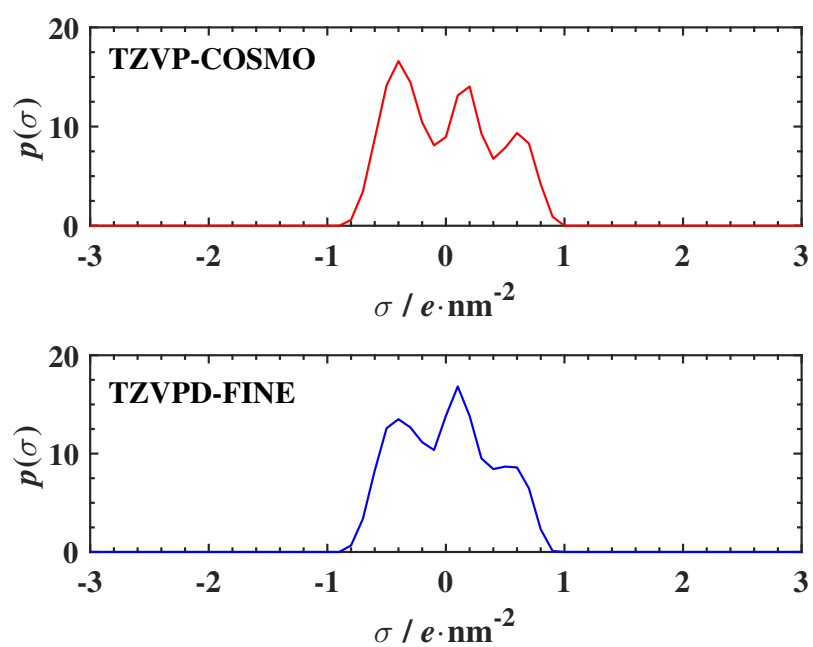
**Figure S193.**  $\sigma$ -profiles of ethylbenzene (CAS-RN: 100-41-4) obtained from screening charge distributions calculated at the BP-TZVP-COSMO level and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



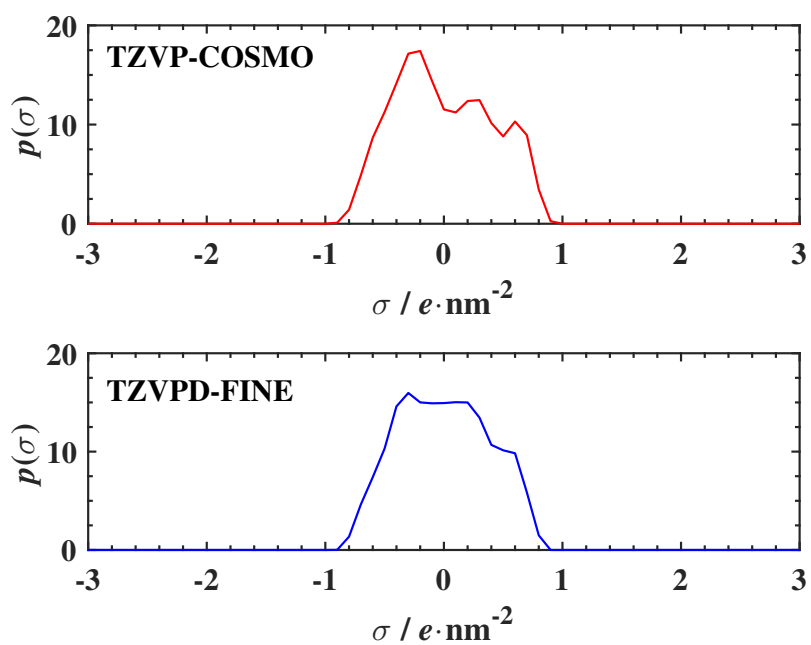
**Figure S194.**  $\sigma$ -profiles of *o*-xylene (CAS-RN: 95-47-6) obtained from screening charge distributions calculated at the BP-TZVP-COSMO level and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



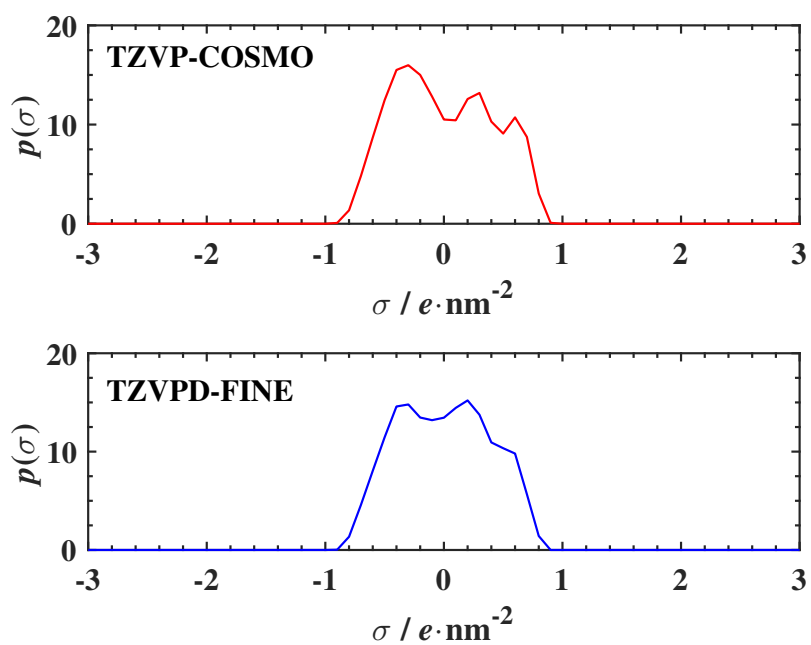
**Figure S195.**  $\sigma$ -profiles of *m*-xylene (CAS-RN: 108-38-3) obtained from screening charge distributions calculated at the BP-TZVP-COSMO level and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



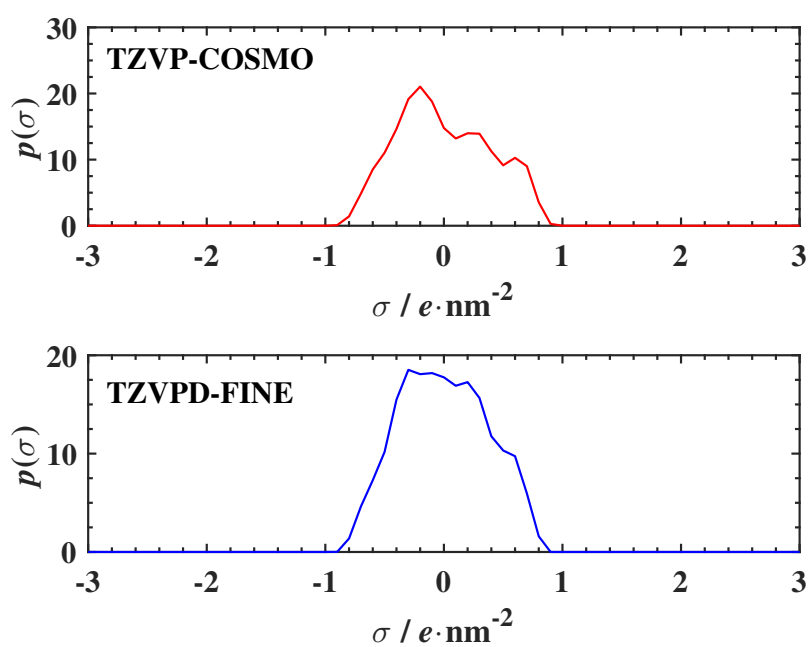
**Figure S196.**  $\sigma$ -profiles of *p*-xylene (CAS-RN: 106-42-3) obtained from screening charge distributions calculated at the BP-TZVP-COSMO level and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



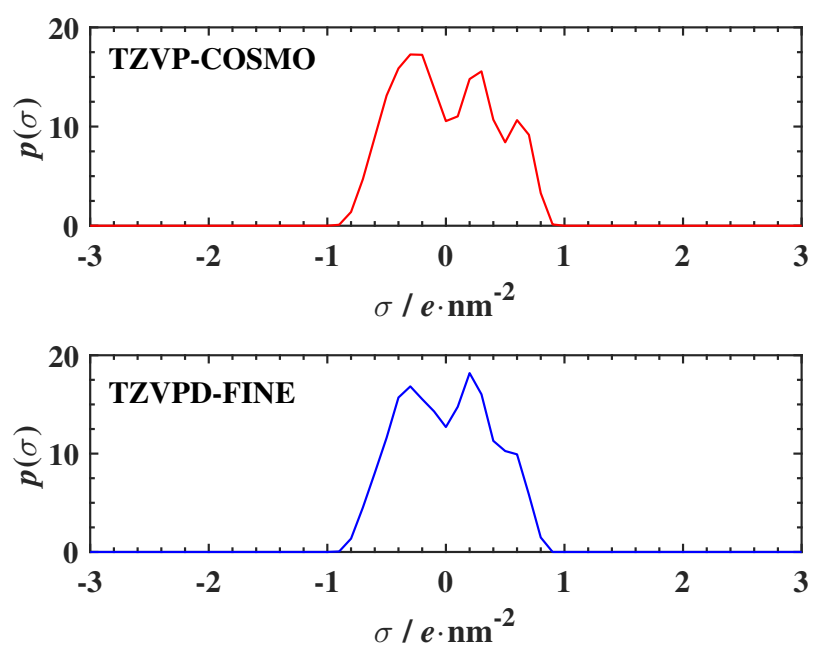
**Figure S197.**  $\sigma$ -profiles of *n*-propylbenzene (CAS-RN: 103-65-1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO level and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



**Figure S198.**  $\sigma$ -profiles of cumene (CAS-RN: 98-82-8) obtained from screening charge distributions calculated at the BP-TZVP-COSMO level and BP-TZVPD-FINE levels. Thick lines are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).

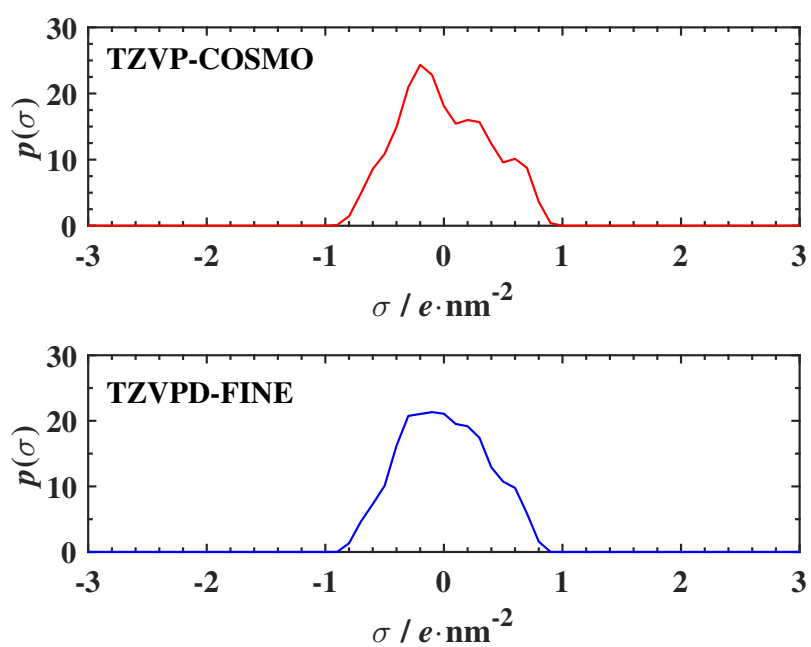


**Figure S199.**  $\sigma$ -profiles of *n*-butylbenzene (CAS-RN: 104-51-8) obtained from screening charge distributions calculated at the BP-TZVP-COSMO level and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).

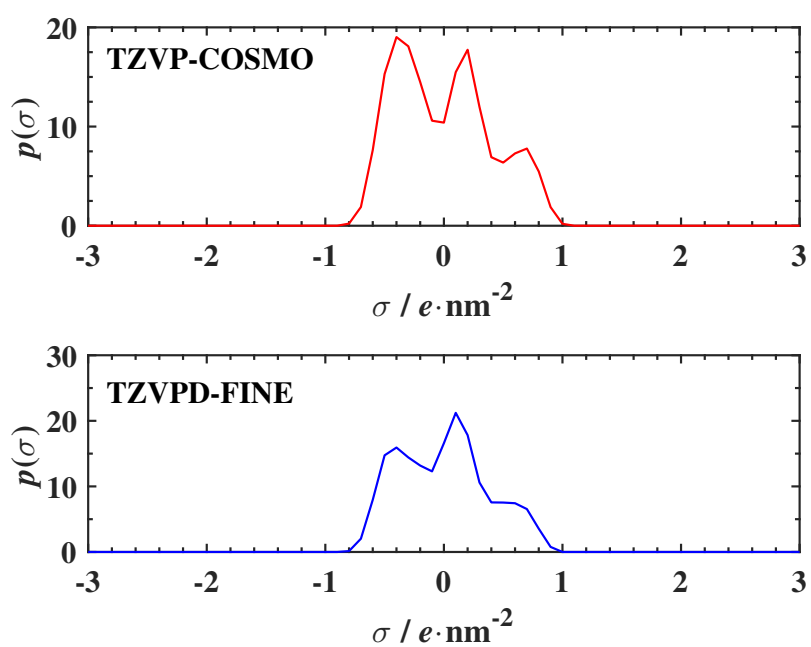


**Figure S200.**  $\sigma$ -profiles of *tert*-butylbenzene (CAS-RN: 98-6-6) obtained from screening charge distributions calculated at the BP-TZVP-COSMO level and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).

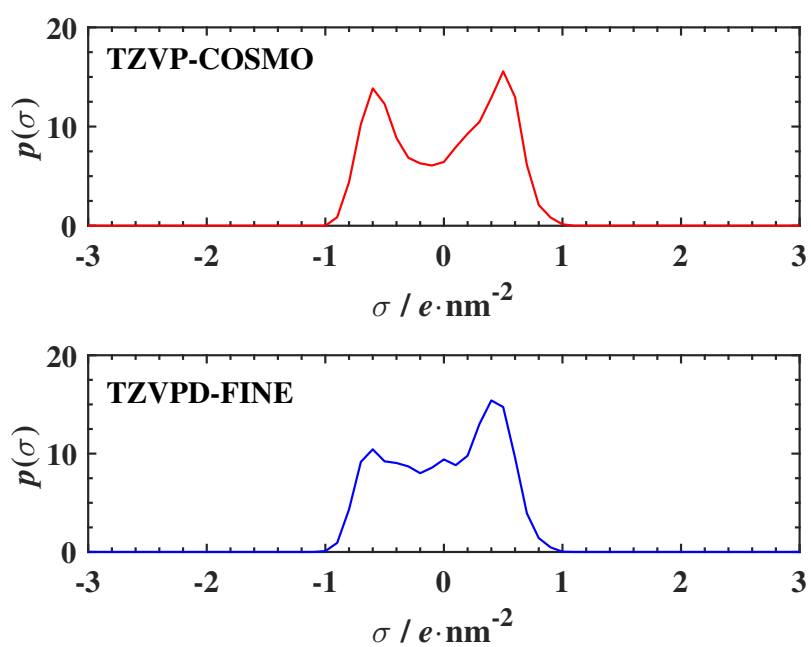




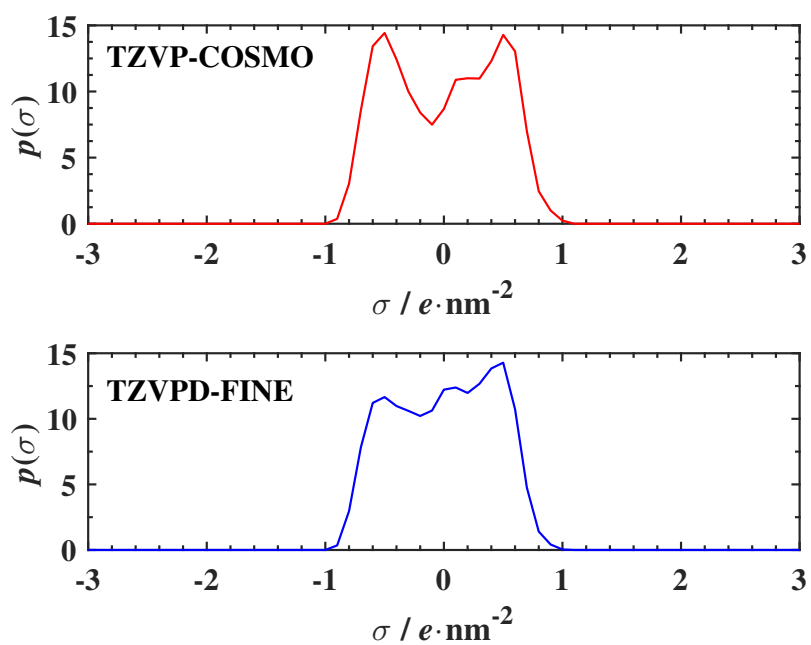
**Figure S201.**  $\sigma$ -profiles of *n*-pentylbenzene (CAS-RN: 538-68-1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO level and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



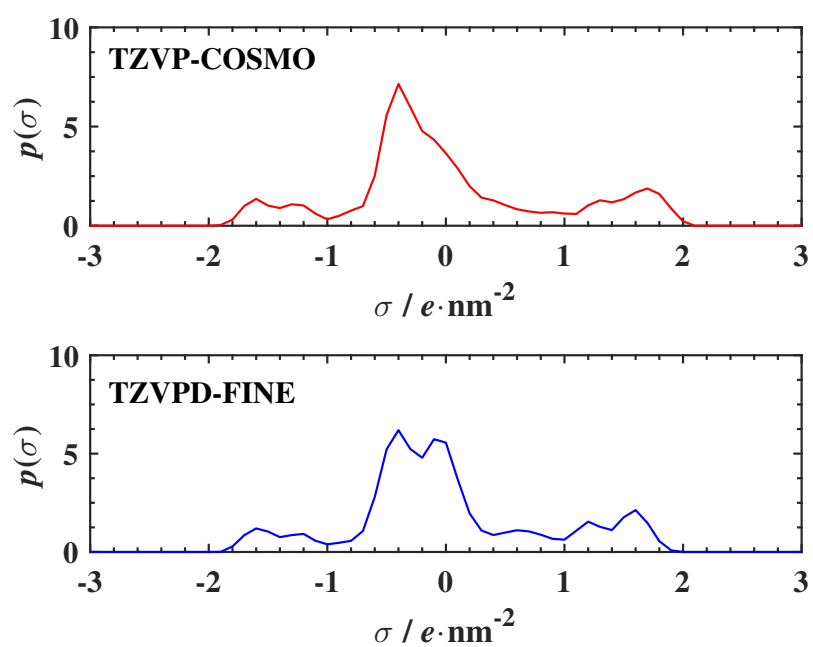
**Figure S202.**  $\sigma$ -profiles of 1,3,5-trimethylbenzene (CAS-RN: 108-67-8) obtained from screening charge distributions calculated at the BP-TZVP-COSMO level and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



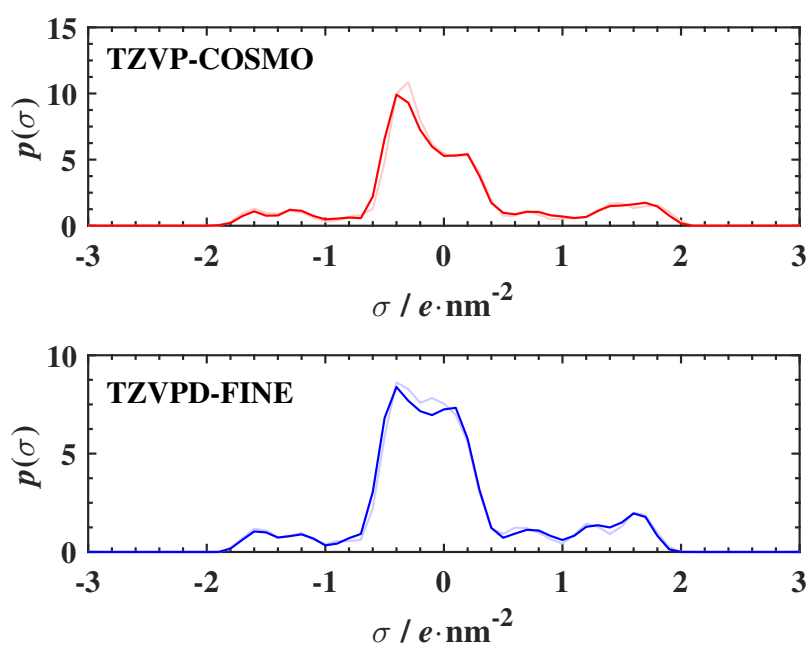
**Figure S203.**  $\sigma$ -profiles of styrene (CAS-RN: 100-42-5) obtained from screening charge distributions calculated at the BP-TZVP-COSMO level and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



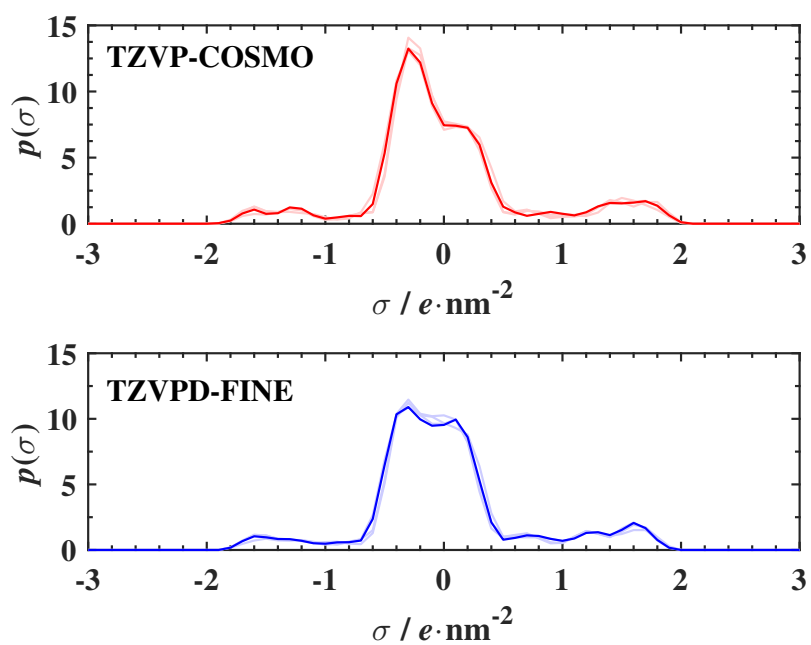
**Figure S204.**  $\sigma$ -profiles of  $\alpha$ -methylstyrene (CAS-RN: 98-83-9) obtained from screening charge distributions calculated at the BP-TZVP-COSMO level and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



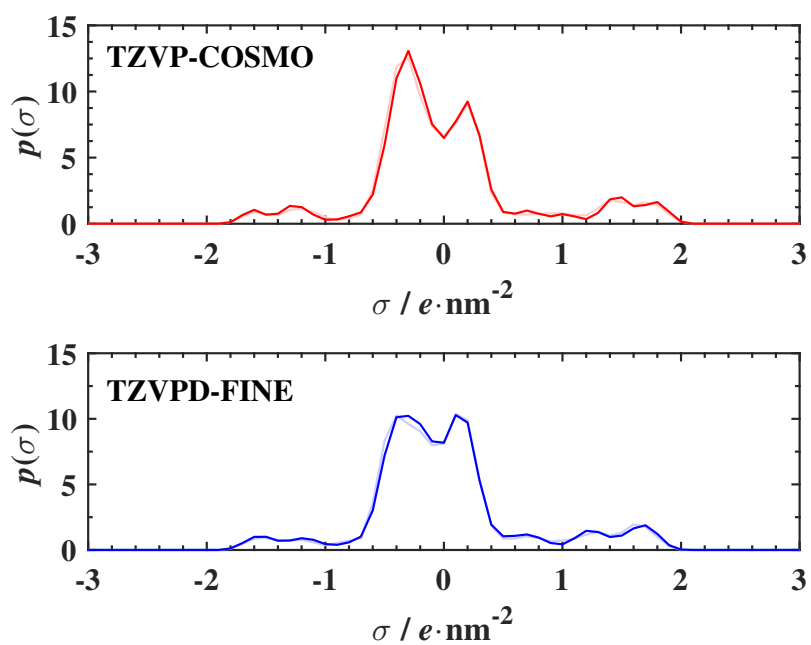
**Figure S205.**  $\sigma$ -profiles of methanol (CAS-RN: 67-56-1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO level and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



**Figure S206.**  $\sigma$ -profiles of ethanol (CAS-RN: 64-17-5) obtained from screening charge distributions calculated at the BP-TZVP-COSMO level and BP-TZVPD-FINE levels. Thick lines are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).

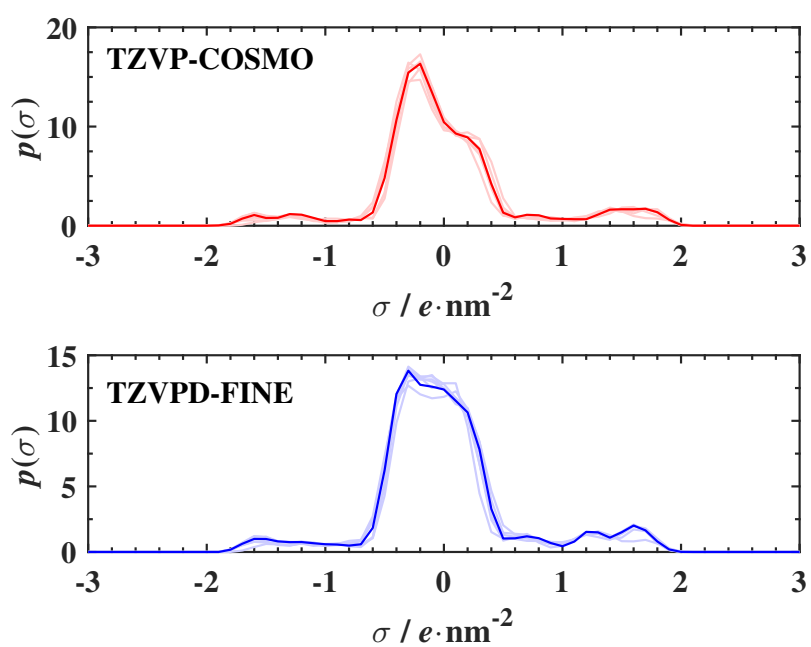


**Figure S207.**  $\sigma$ -profiles of 1-propanol (CAS-RN: 71-23-8) obtained from screening charge distributions calculated at the BP-TZVP-COSMO level and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).

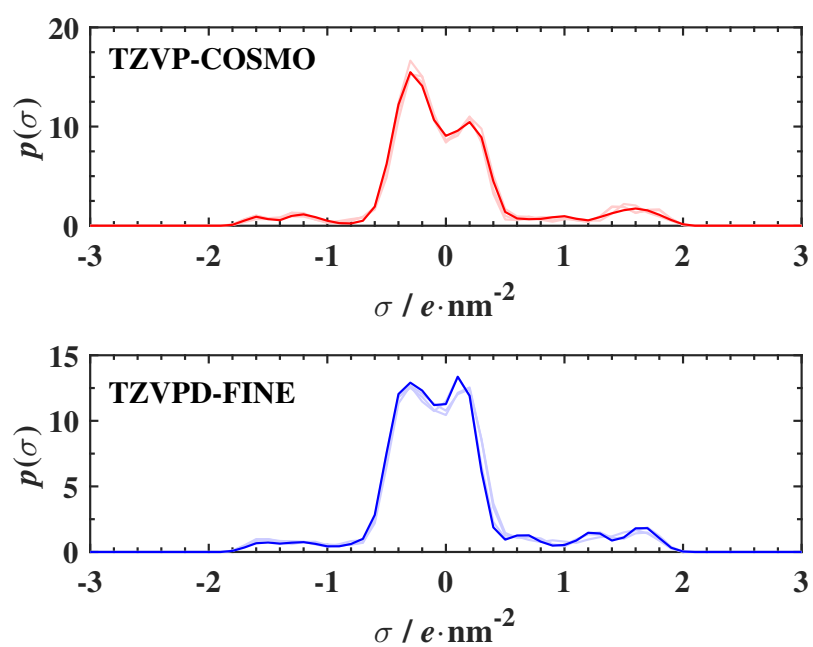


**Figure S208.**  $\sigma$ -profiles of 2-propanol (CAS-RN: 67-63-0) obtained from screening charge distributions calculated at the BP-TZVP-COSMO level and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).

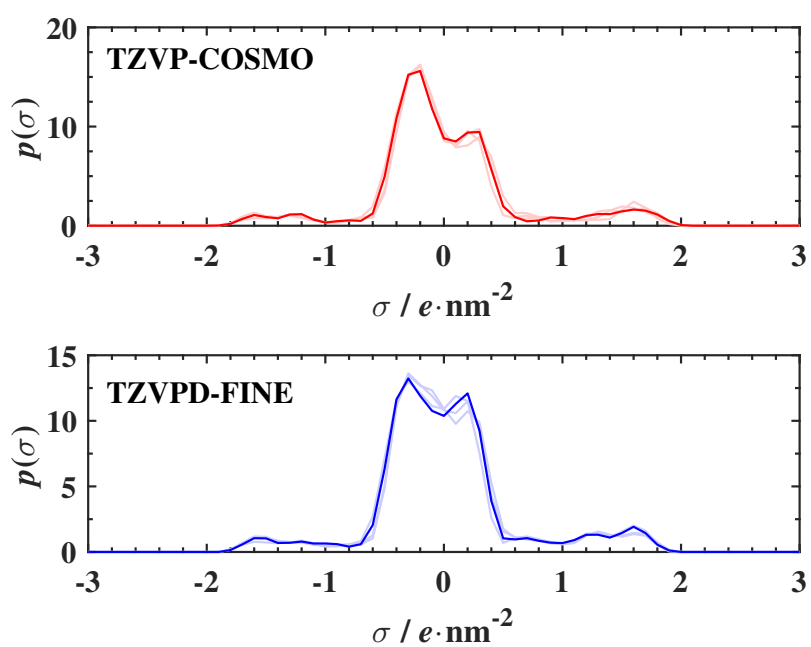




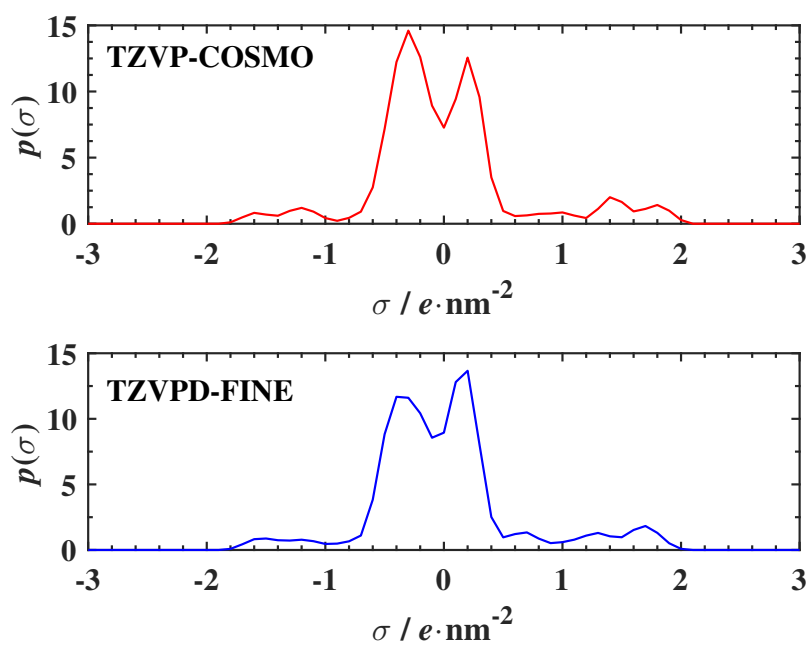
**Figure S209.**  $\sigma$ -profiles of 1-butanol (CAS-RN: 71-36-3) obtained from screening charge distributions calculated at the BP-TZVP-COSMO level and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



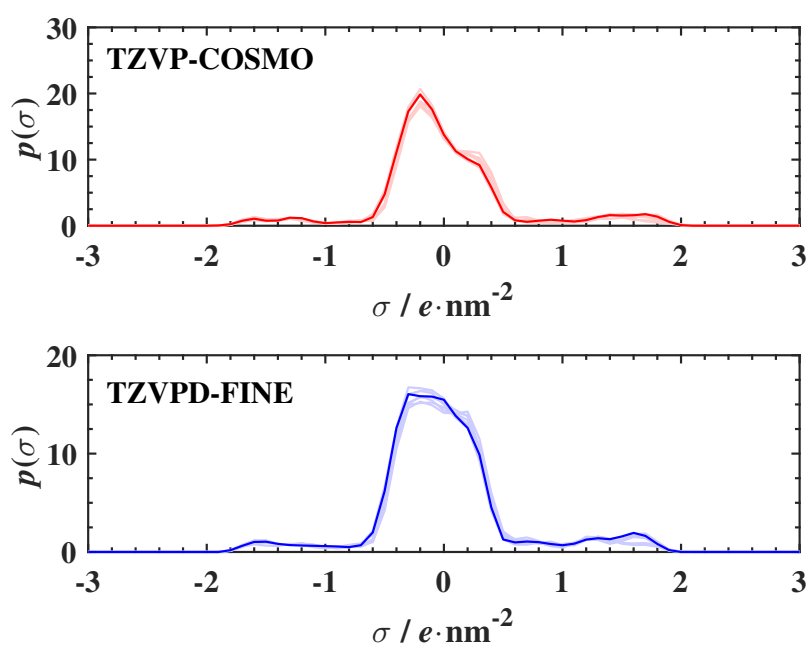
**Figure S210.**  $\sigma$ -profiles of 2-butanol (CAS-RN: 78-92-2) obtained from screening charge distributions calculated at the BP-TZVP-COSMO level and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



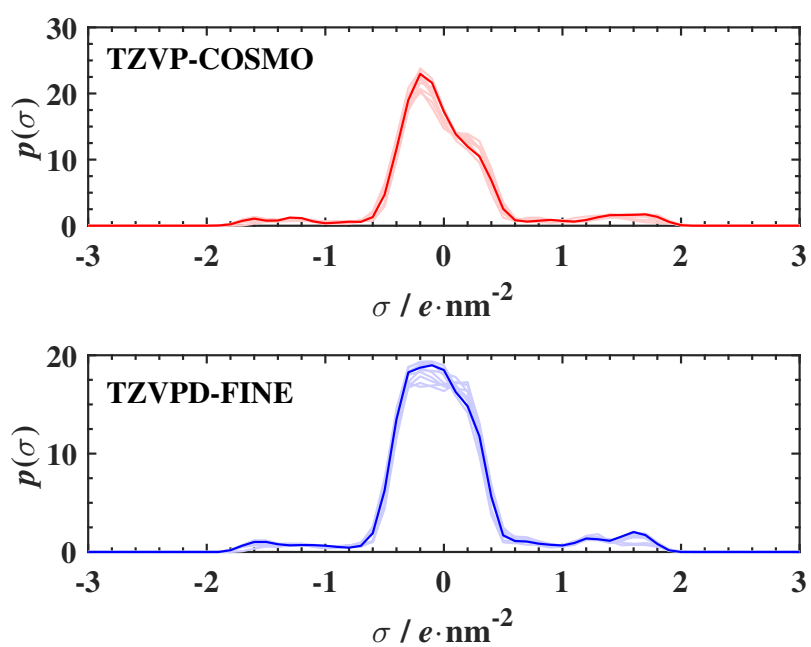
**Figure S211.**  $\sigma$ -profiles of 2-methyl-1-propanol (CAS-RN: 78-83-1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO level and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



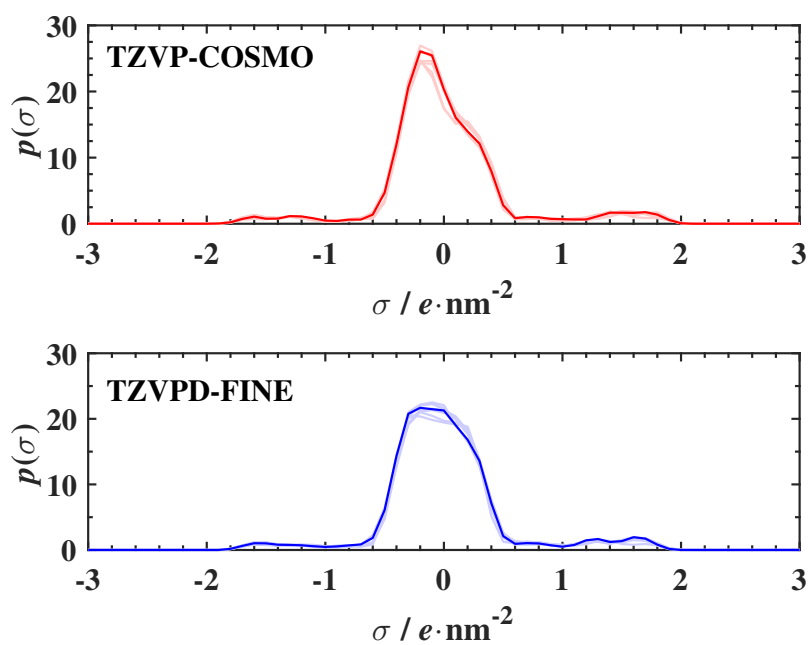
**Figure S212.**  $\sigma$ -profiles of *tert*-butanol (CAS-RN: 75-65-0) obtained from screening charge distributions calculated at the BP-TZVP-COSMO level and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



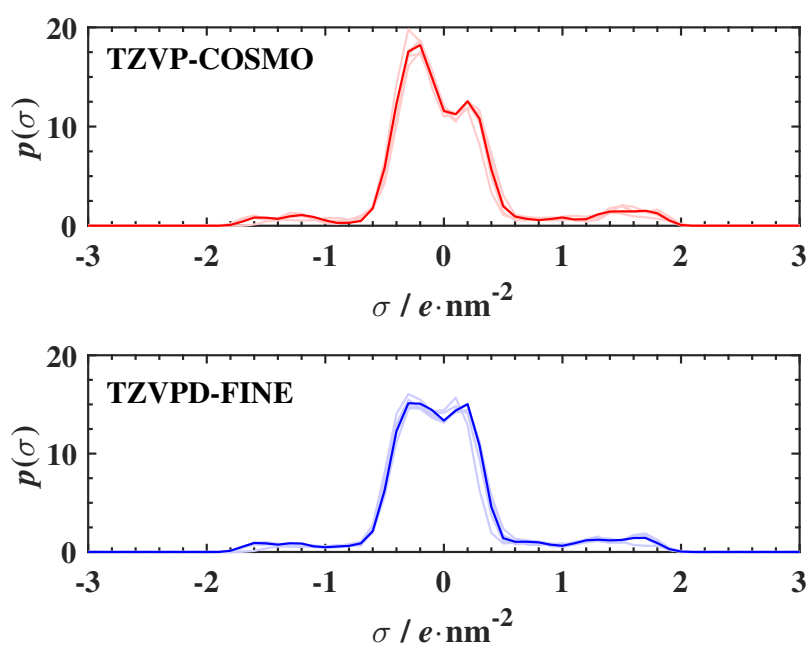
**Figure S213.**  $\sigma$ -profiles of 1-pentanol (CAS-RN: 71-41-0) obtained from screening charge distributions calculated at the BP-TZVP-COSMO level and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



**Figure S214.**  $\sigma$ -profiles of 1-hexanol (CAS-RN: 111-27-3) obtained from screening charge distributions calculated at the BP-TZVP-COSMO level and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).

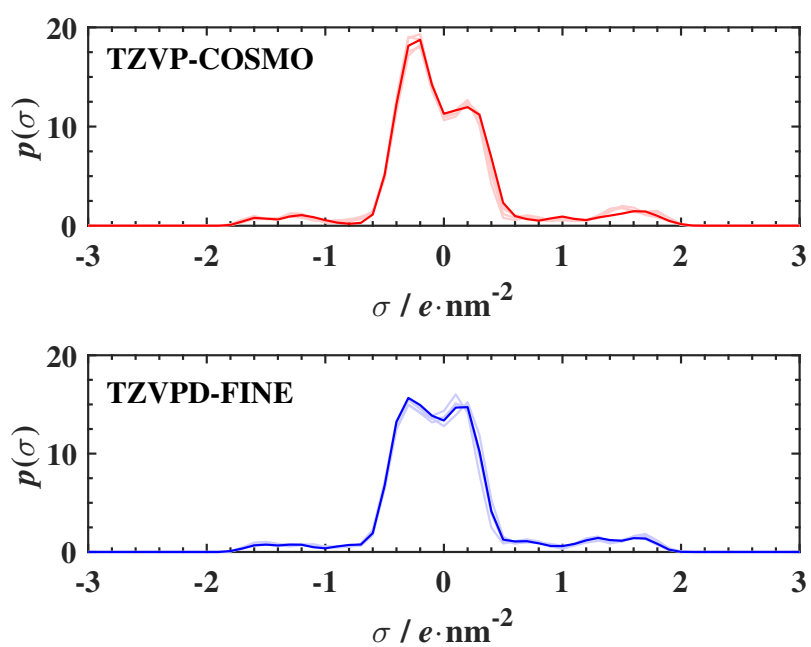


**Figure S215.**  $\sigma$ -profiles of 1-heptanol (CAS-RN: 111-70-6) obtained from screening charge distributions calculated at the BP-TZVP-COSMO level and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).

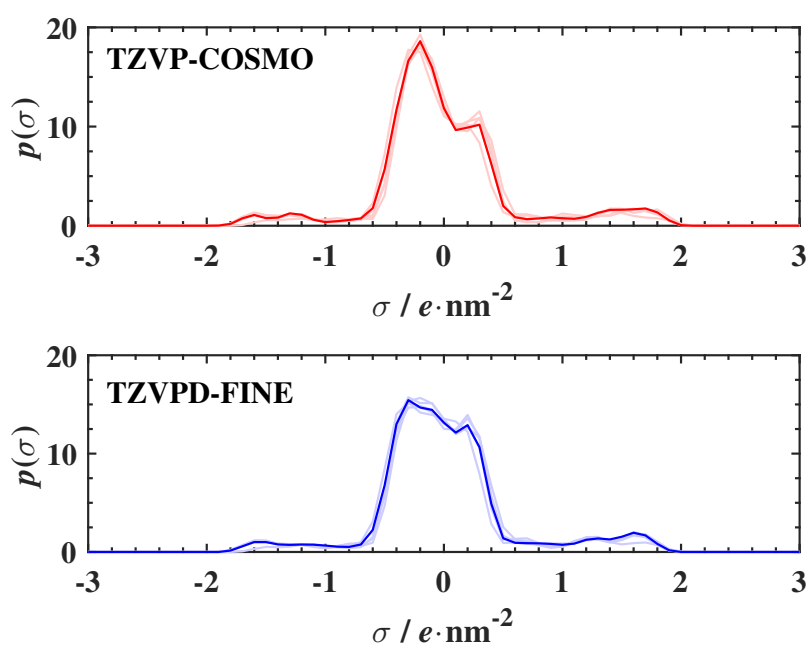


**Figure S216.**  $\sigma$ -profiles of 2-pentanol (CAS-RN: 6032-29-7) obtained from screening charge distributions calculated at the BP-TZVP-COSMO level and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).

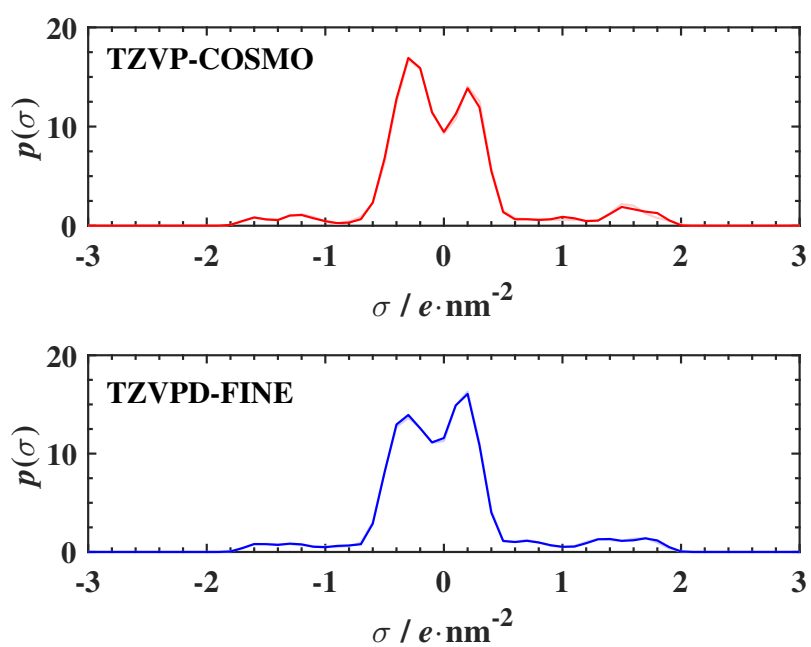




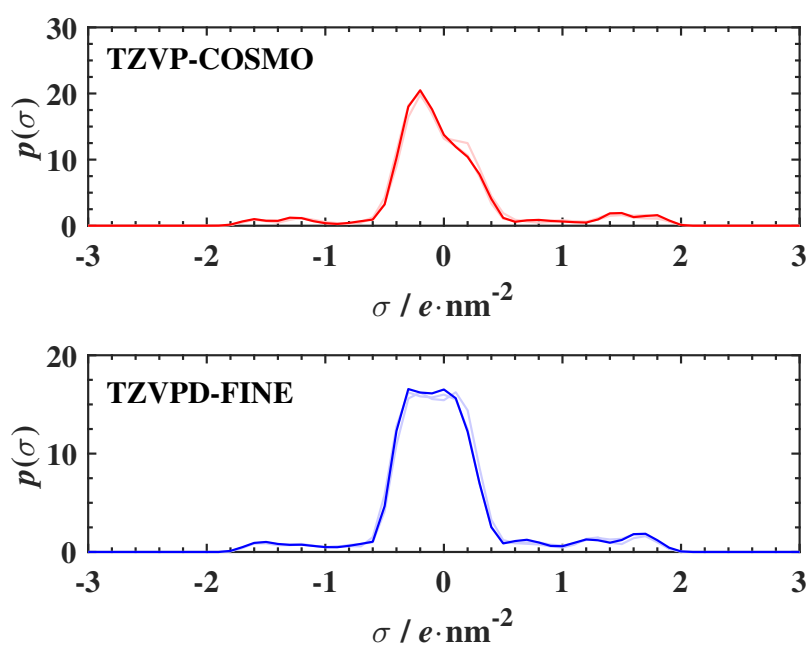
**Figure S217.**  $\sigma$ -profiles of 3-pentanol (CAS-RN: 584-2-1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO level and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



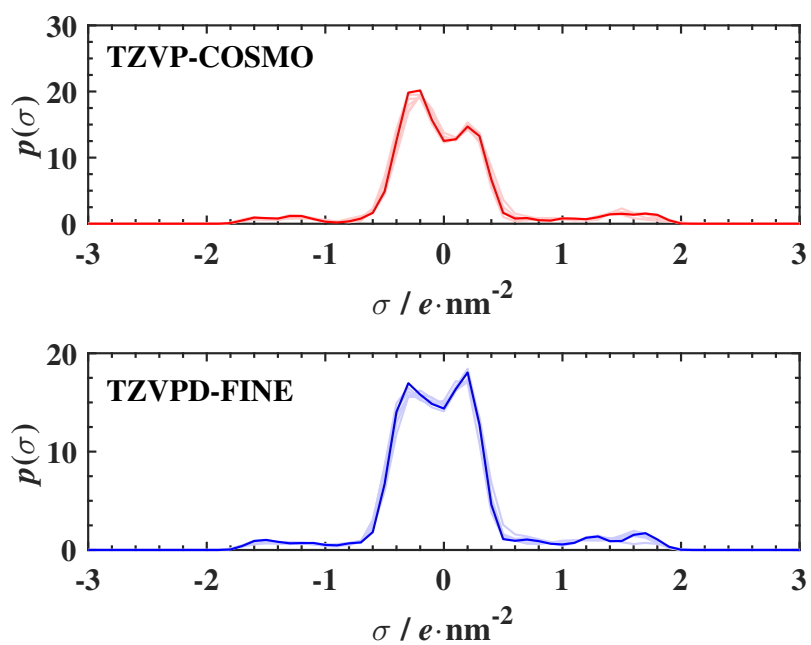
**Figure S218.**  $\sigma$ -profiles of 3-methyl-1-butanol (CAS-RN: 123-51-3) obtained from screening charge distributions calculated at the BP-TZVP-COSMO level and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



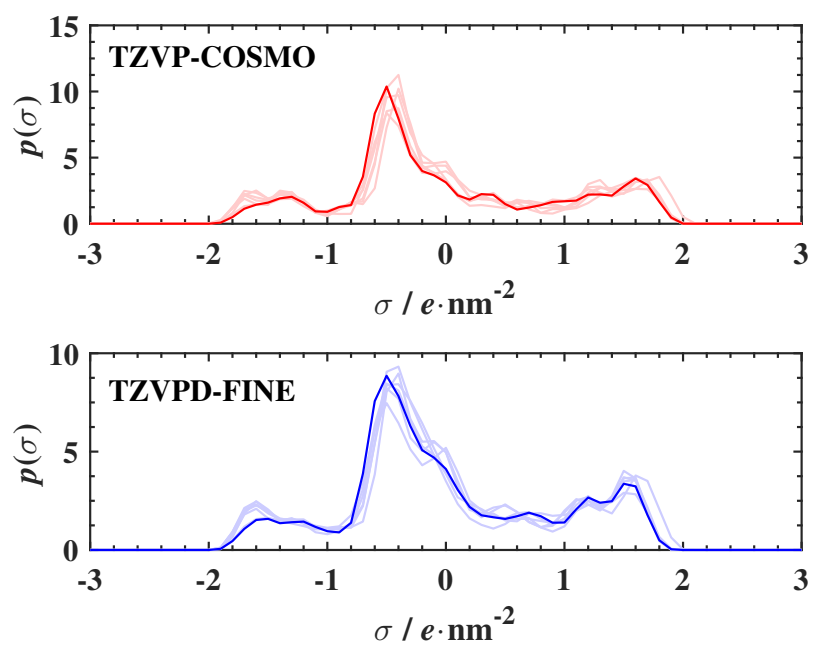
**Figure S219.**  $\sigma$ -profiles of 2-methyl-2-butanol (CAS-RN: 75-85-4) obtained from screening charge distributions calculated at the BP-TZVP-COSMO level and BP-TZVPD-FINE levels. Thick lines are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



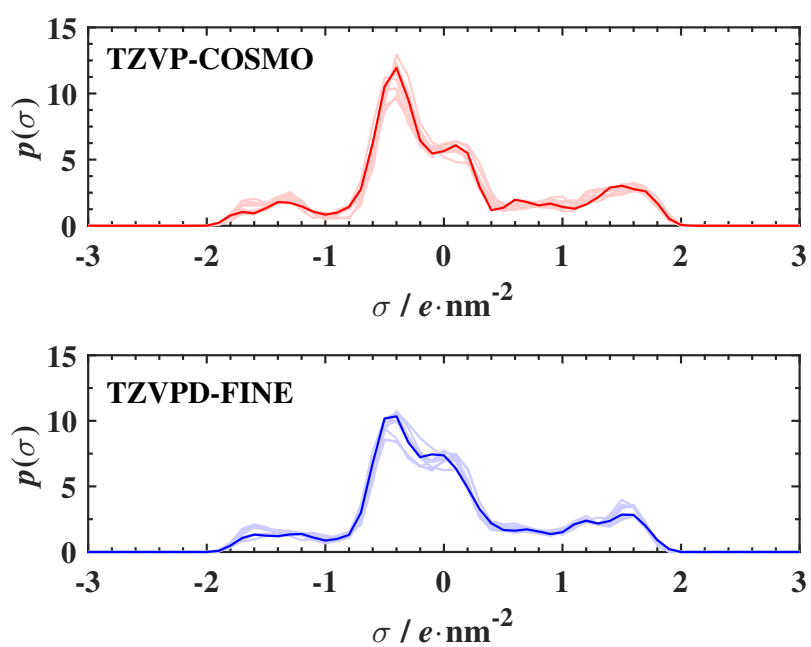
**Figure S220.**  $\sigma$ -profiles of cyclohexanol (CAS-RN: 108-93-0) obtained from screening charge distributions calculated at the BP-TZVP-COSMO level and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



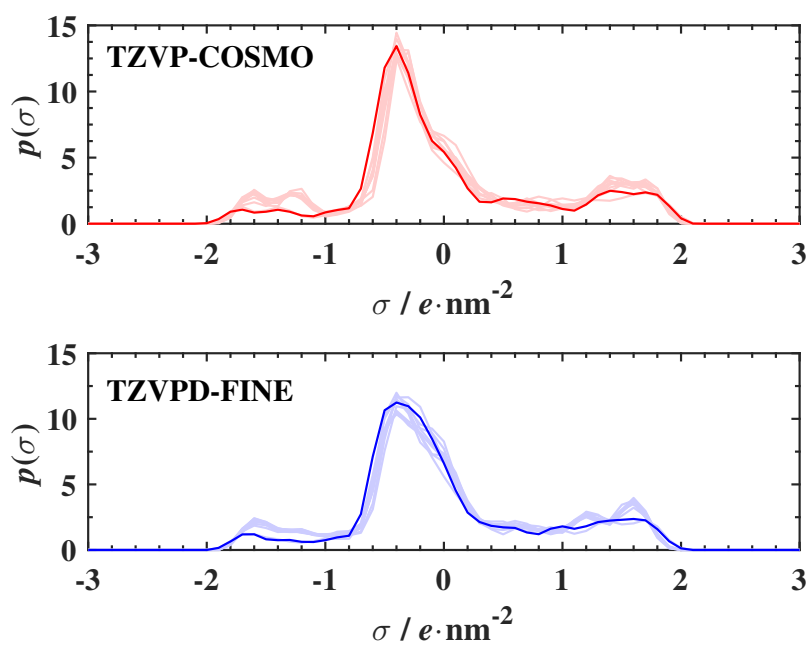
**Figure S221.**  $\sigma$ -profiles of 2-methyl-2-pentanol (CAS-RN: 590-36-3) obtained from screening charge distributions calculated at the BP-TZVP-COSMO level and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



**Figure S222.**  $\sigma$ -profiles of 1,2-ethanediol (CAS-RN: 107-21-1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO level and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).

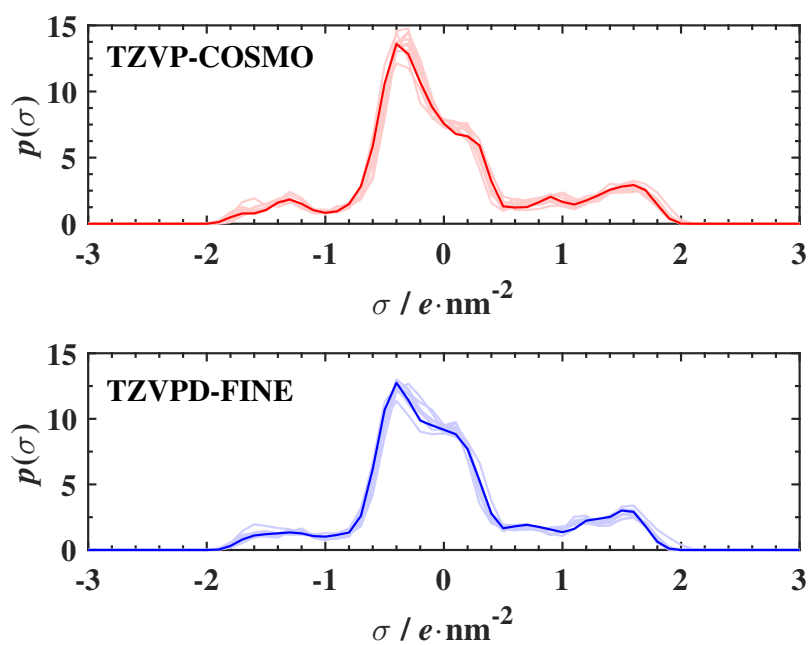


**Figure S223.**  $\sigma$ -profiles of 1,2-Propanediol (CAS-RN: 57-55-6) obtained from screening charge distributions calculated at the BP-TZVP-COSMO level and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).

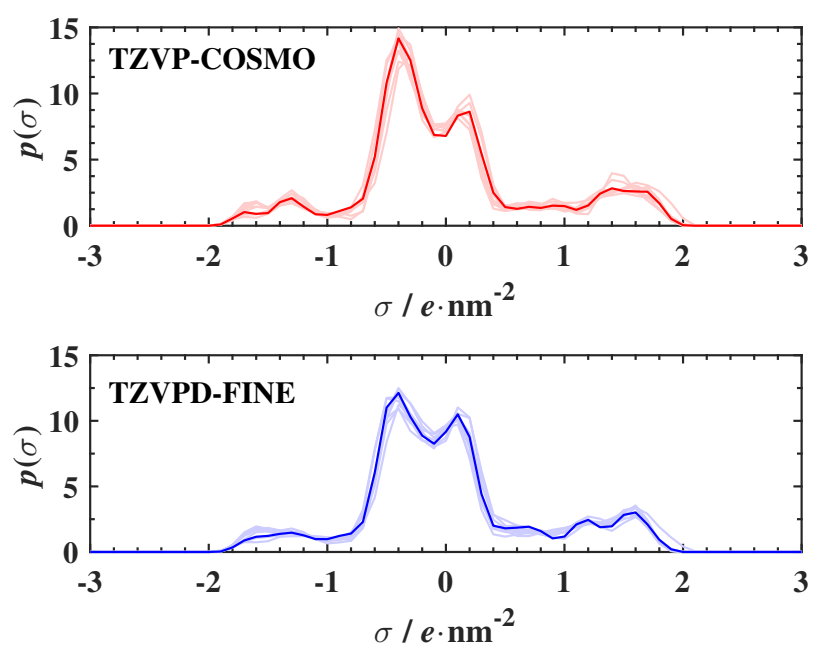


**Figure S224.**  $\sigma$ -profiles of 1,3-Propanediol (CAS-RN: 504-63-2) obtained from screening charge distributions calculated at the BP-TZVP-COSMO level and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).

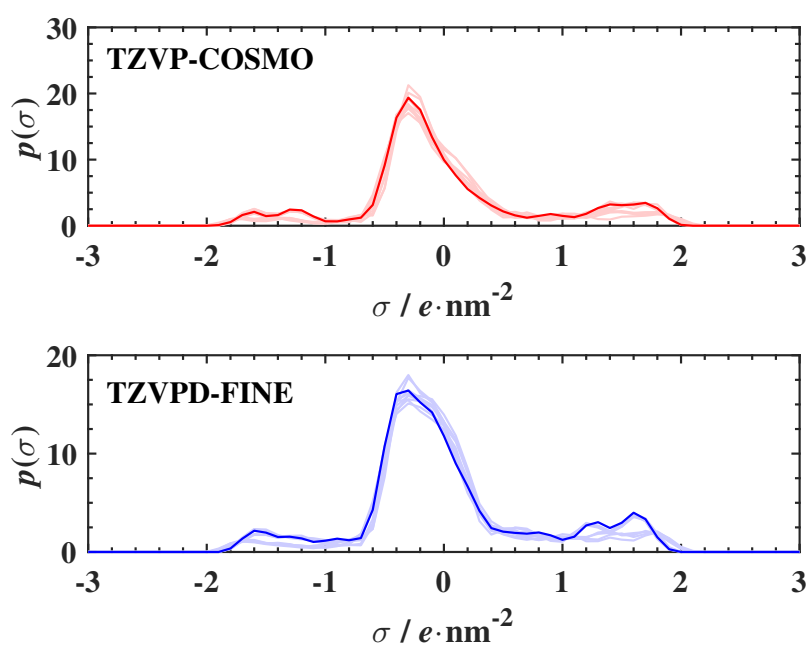




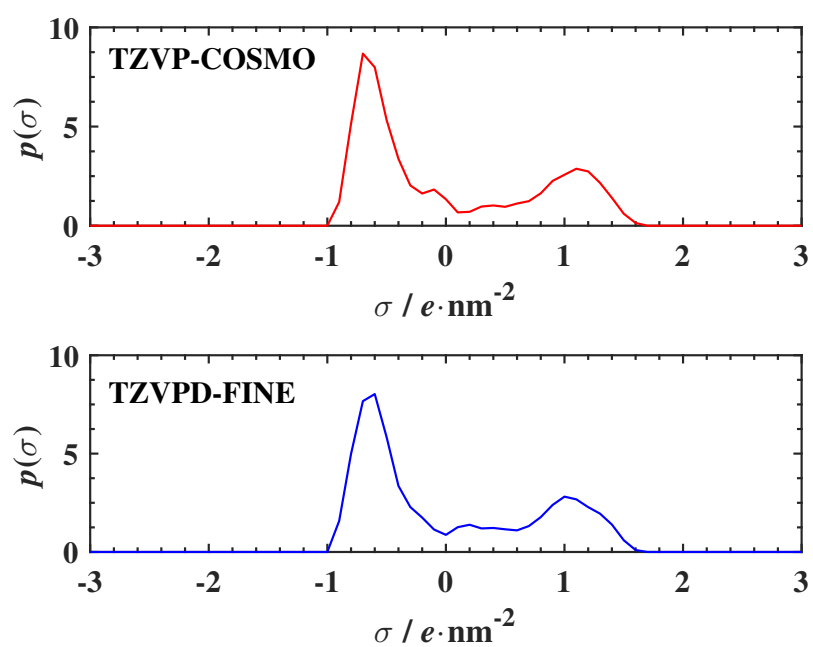
**Figure S225.**  $\sigma$ -profiles of 1,2-Butanediol (CAS-RN: 584-3-2) obtained from screening charge distributions calculated at the BP-TZVP-COSMO level and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



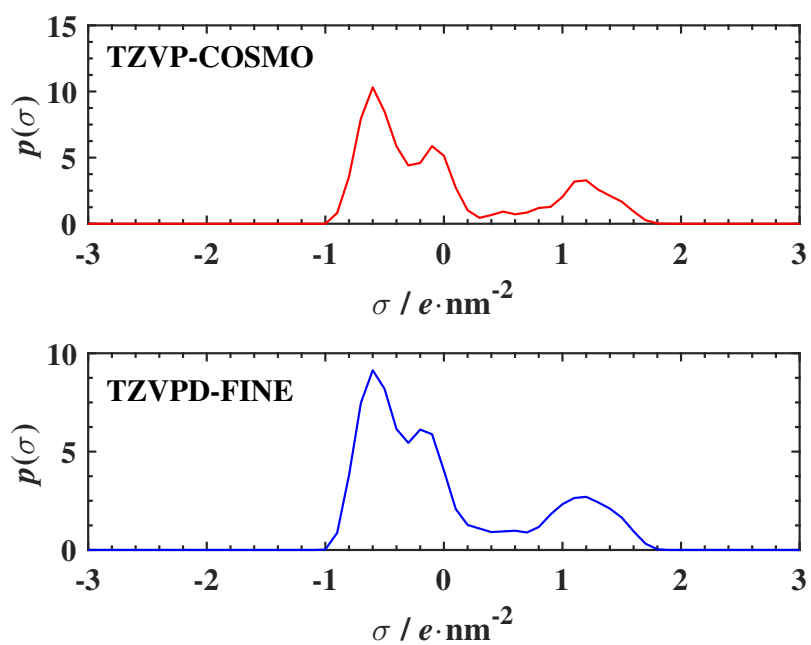
**Figure S226.**  $\sigma$ -profiles of 2,3-Butanediol (CAS-RN: 513-85-9) obtained from screening charge distributions calculated at the BP-TZVP-COSMO level and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



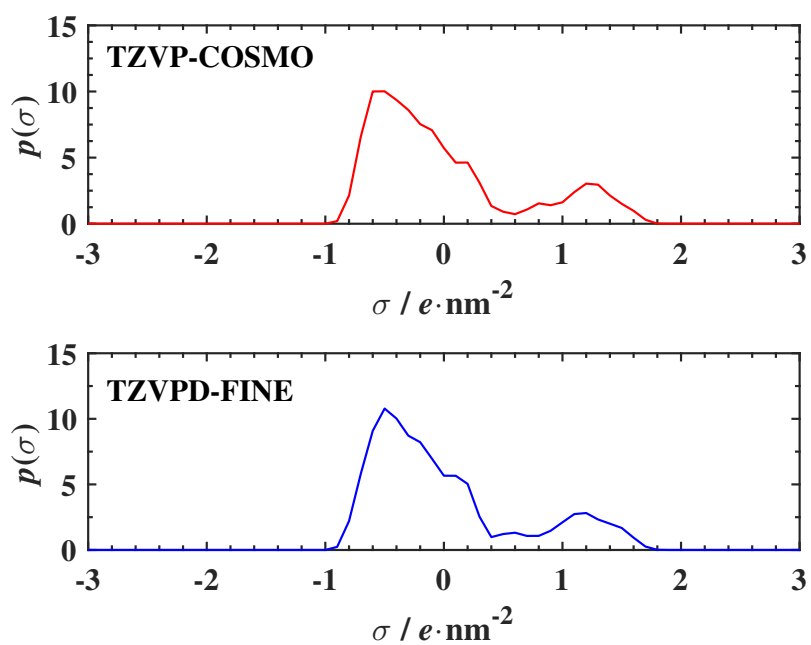
**Figure S227.**  $\sigma$ -profiles of 1,5-Pentanediol (CAS-RN: 111-29-5) obtained from screening charge distributions calculated at the BP-TZVP-COSMO level and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



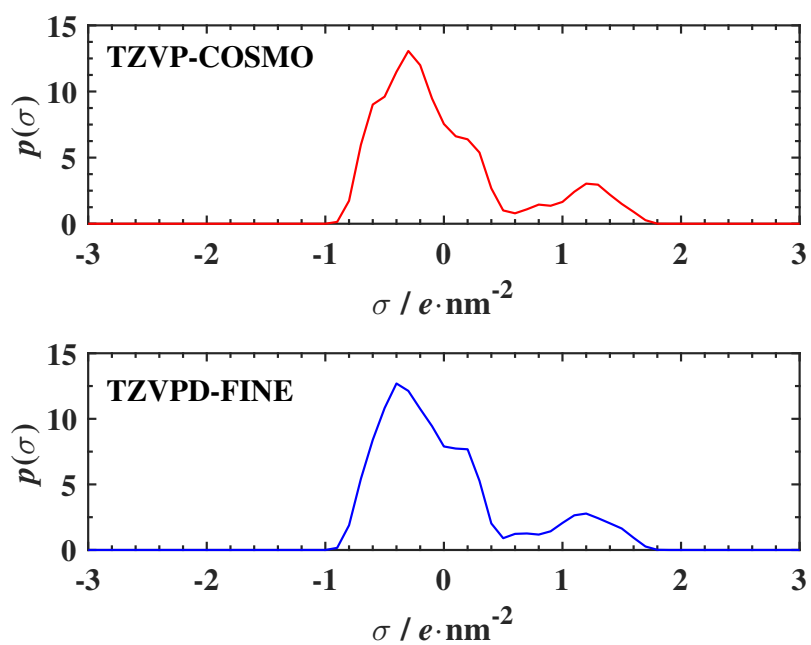
**Figure S228.**  $\sigma$ -profiles of methanal (CAS-RN: 50-0-0) obtained from screening charge distributions calculated at the BP-TZVP-COSMO level and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



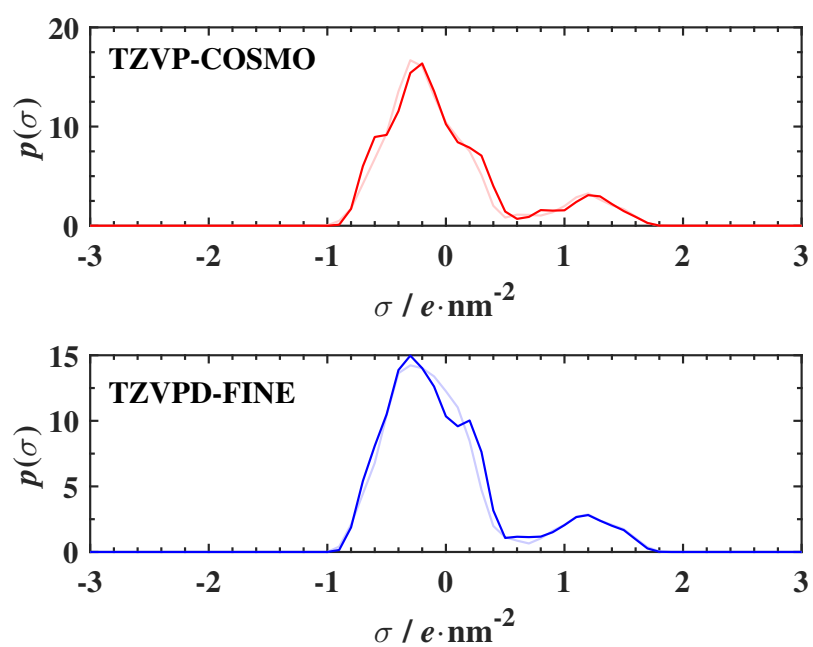
**Figure S229.**  $\sigma$ -profiles of ethanal (CAS-RN: 75-7-0) obtained from screening charge distributions calculated at the BP-TZVP-COSMO level and BP-TZVPD-FINE levels. Thick lines are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



**Figure S230.**  $\sigma$ -profiles of propanal (CAS-RN: 123-38-6) obtained from screening charge distributions calculated at the BP-TZVP-COSMO level and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).

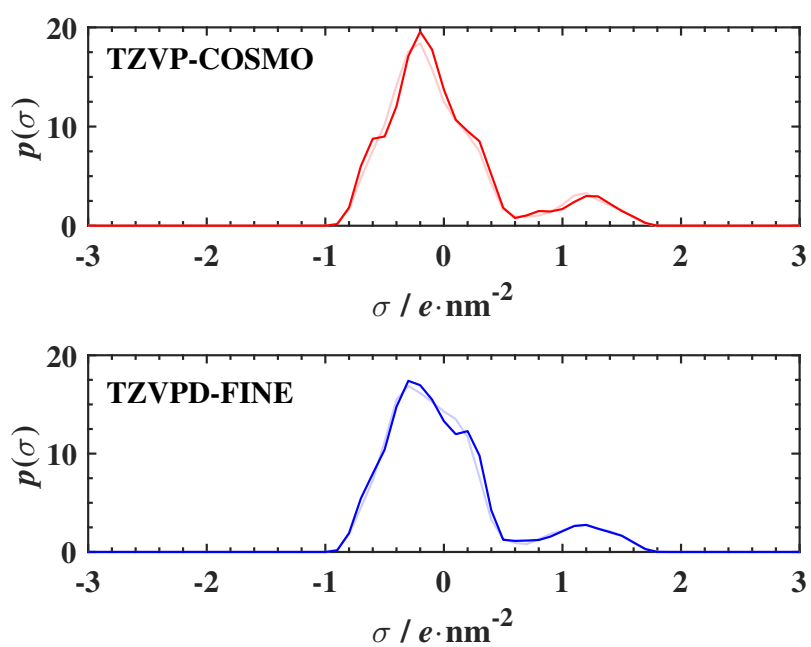


**Figure S231.**  $\sigma$ -profiles of butanal (CAS-RN: 123-72-8) obtained from screening charge distributions calculated at the BP-TZVP-COSMO level and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).

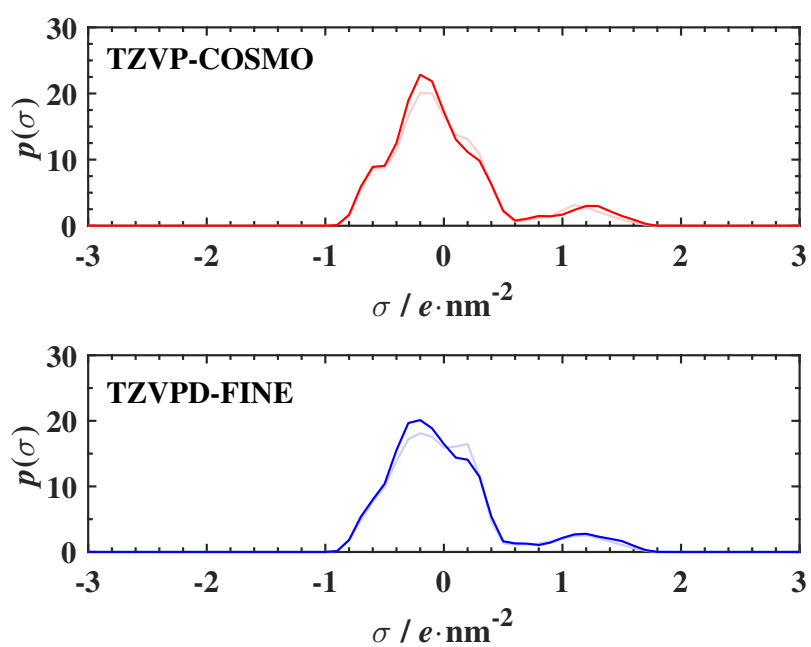


**Figure S232.**  $\sigma$ -profiles of pentanal (CAS-RN: 110-62-3) obtained from screening charge distributions calculated at the BP-TZVP-COSMO level and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).

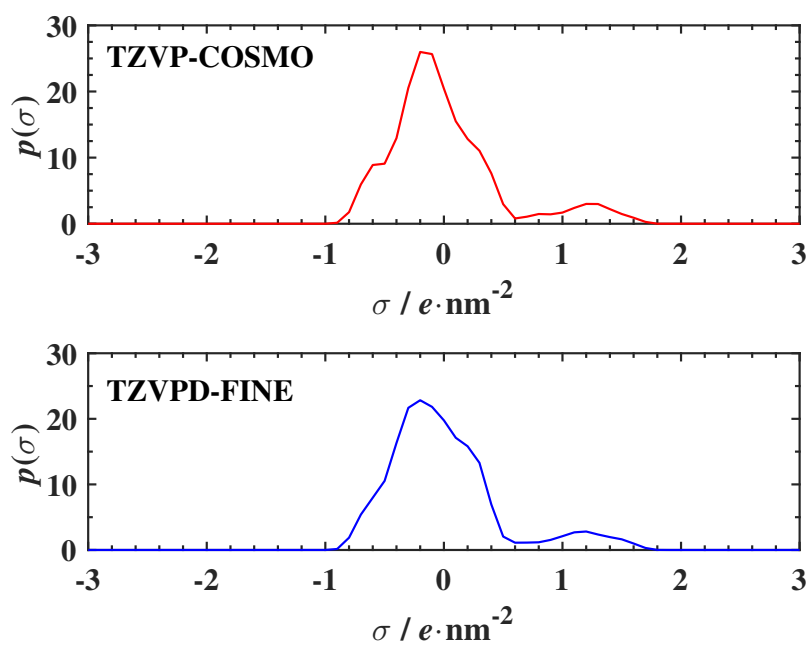




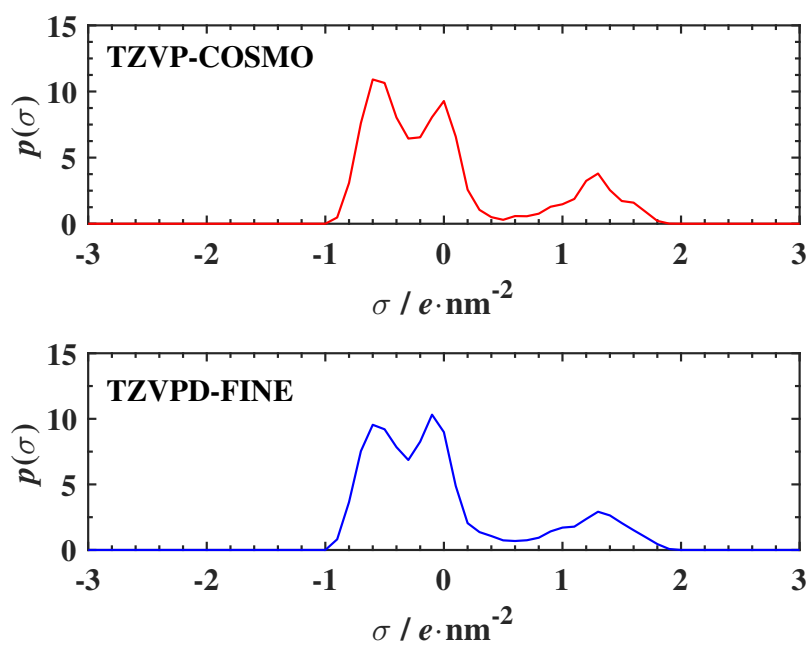
**Figure S233.**  $\sigma$ -profiles of hexanal (CAS-RN: 66-25-1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO level and BP-TZVPD-FINE levels. Thick lines are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



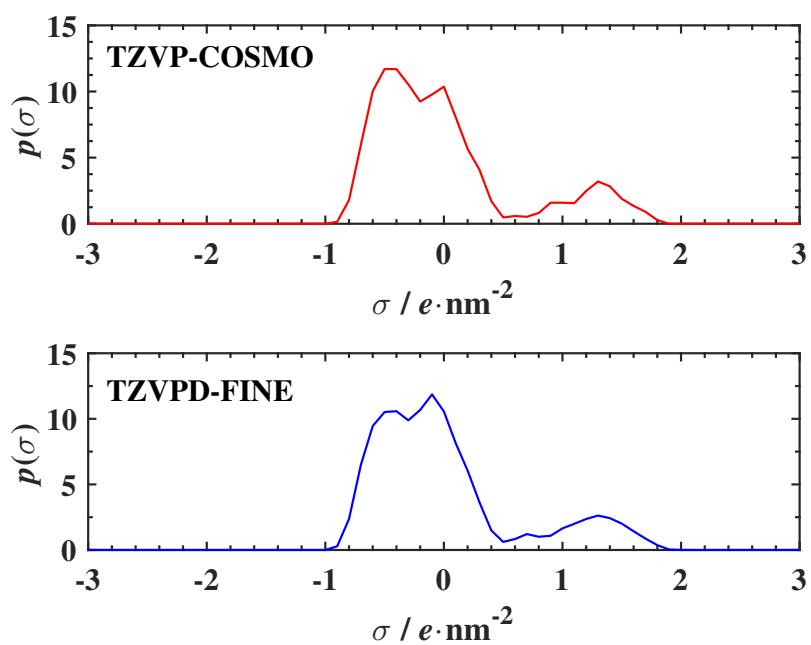
**Figure S234.**  $\sigma$ -profiles of heptanal (CAS-RN: 111-71-7) obtained from screening charge distributions calculated at the BP-TZVP-COSMO level and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



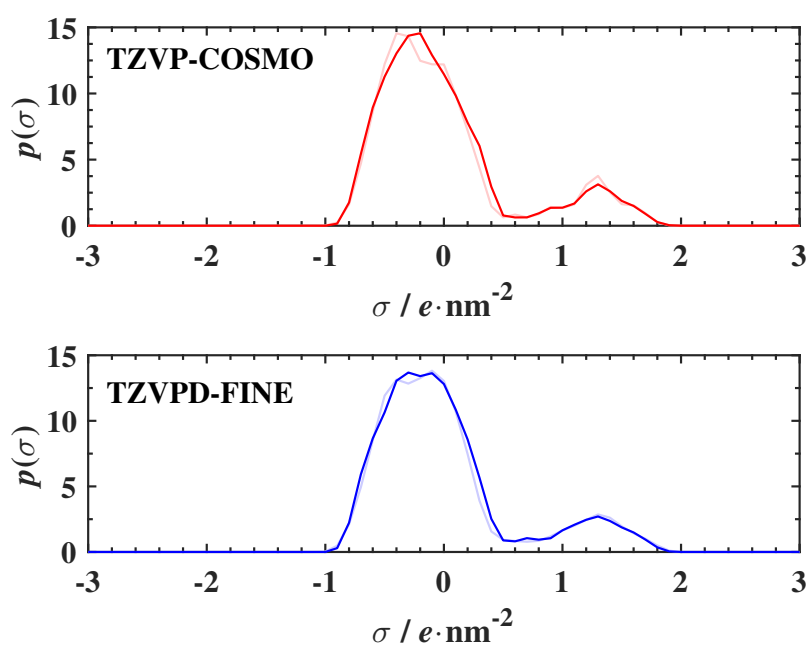
**Figure S235.**  $\sigma$ -profiles of octanal (CAS-RN: 124-13-0) obtained from screening charge distributions calculated at the BP-TZVP-COSMO level and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



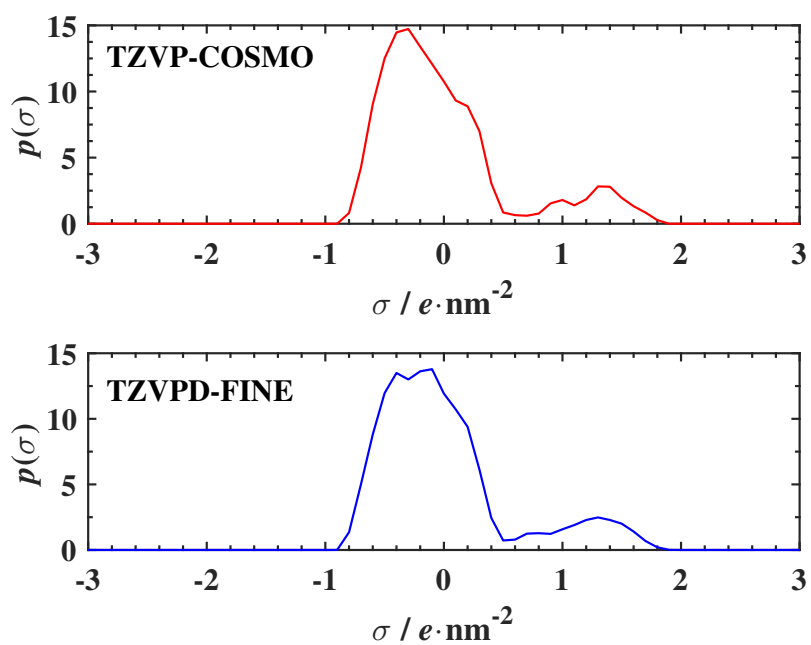
**Figure S236.**  $\sigma$ -profiles of acetone (CAS-RN: 67-64-1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO level and BP-TZVPD-FINE levels. Thick lines are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



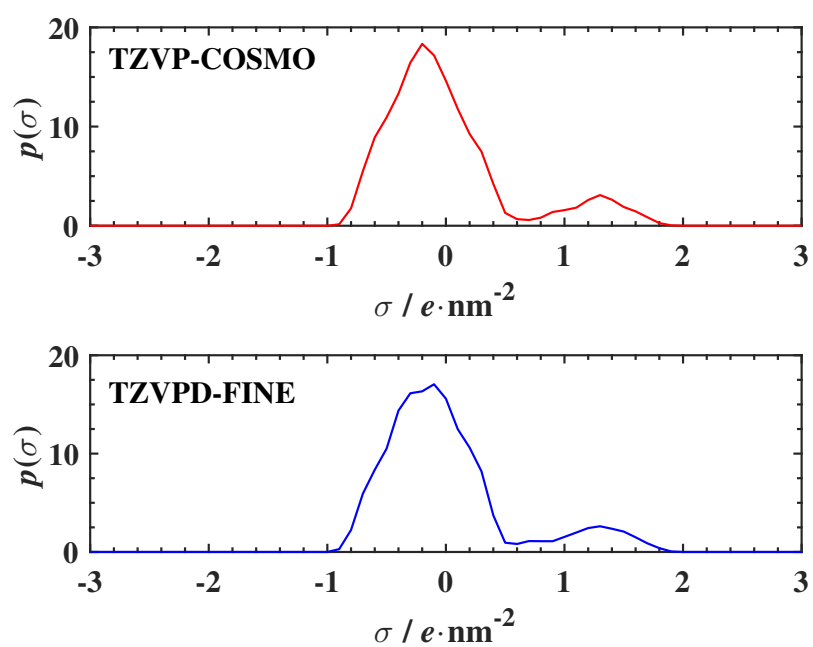
**Figure S237.**  $\sigma$ -profiles of butanone (CAS-RN: 78-93-3) obtained from screening charge distributions calculated at the BP-TZVP-COSMO level and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



**Figure S238.**  $\sigma$ -profiles of 2-pentanone (CAS-RN: 107-87-9) obtained from screening charge distributions calculated at the BP-TZVP-COSMO level and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).

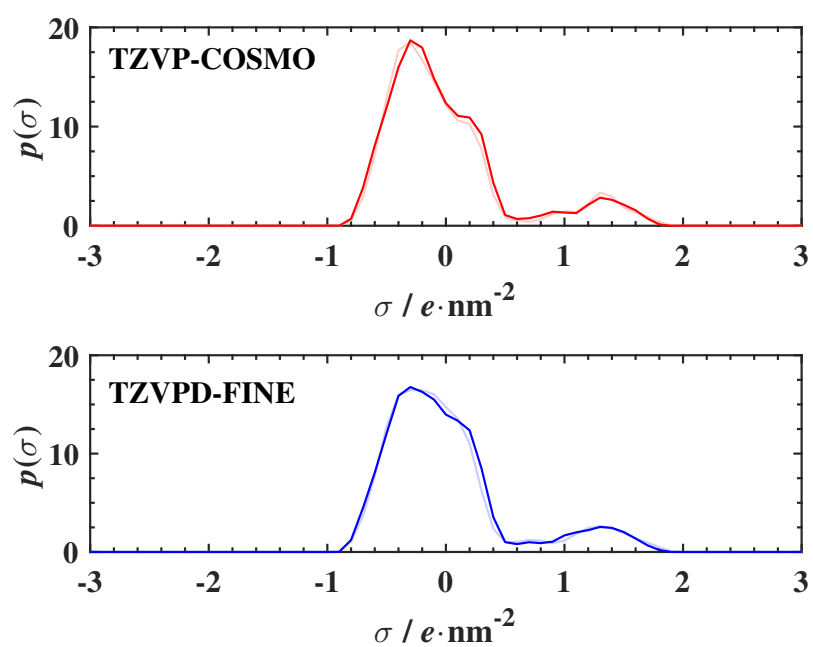


**Figure S239.**  $\sigma$ -profiles of 3-pentanone (CAS-RN: 96-22-0) obtained from screening charge distributions calculated at the BP-TZVP-COSMO level and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).

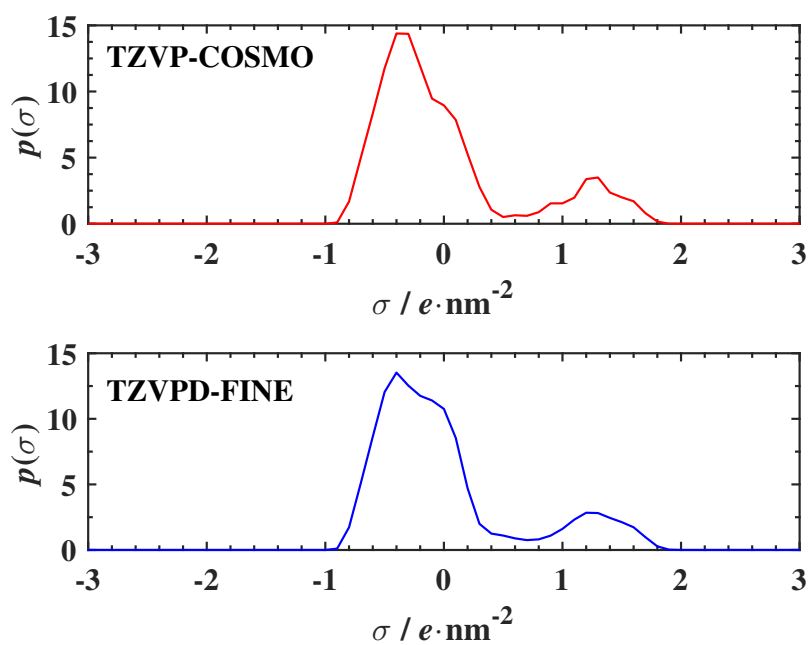


**Figure S240.**  $\sigma$ -profiles of 2-hexanone (CAS-RN: 591-78-6) obtained from screening charge distributions calculated at the BP-TZVP-COSMO level and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).

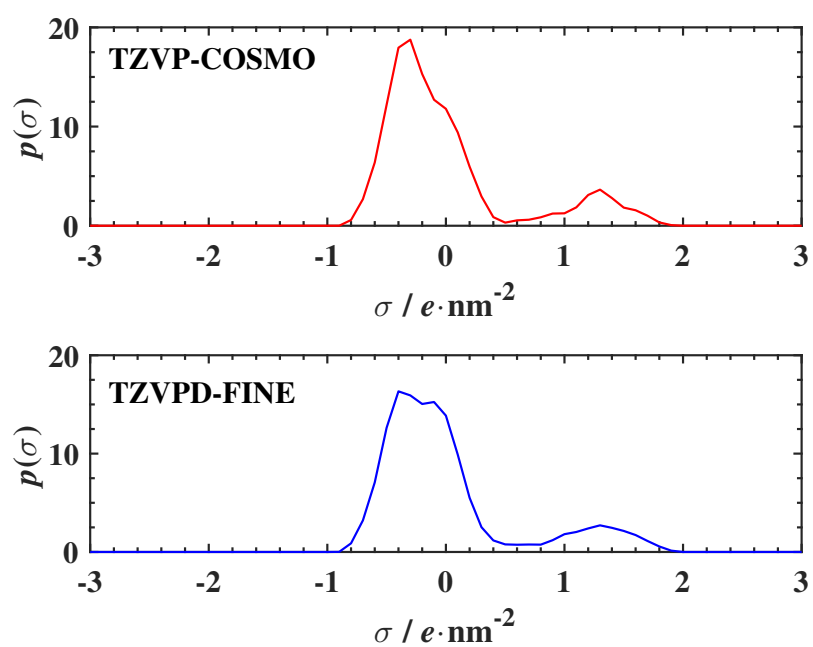




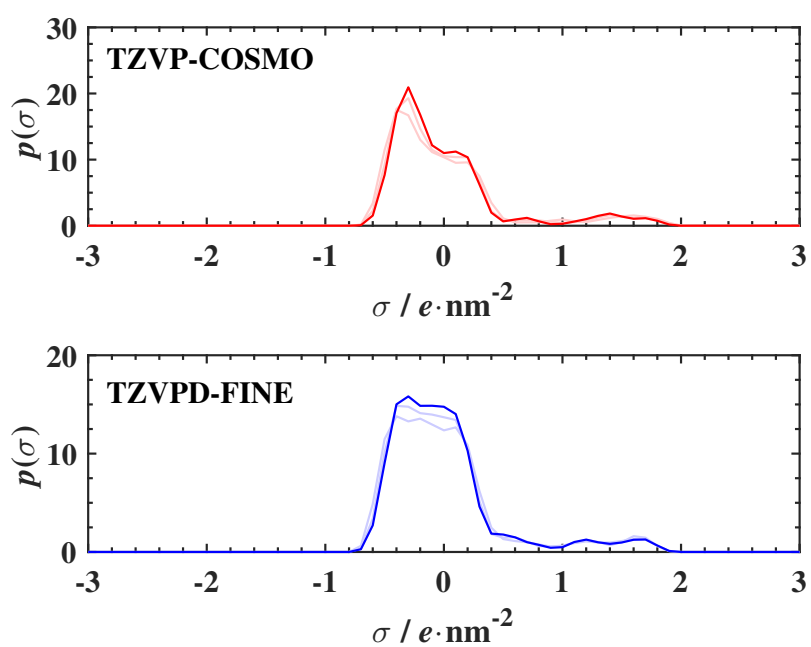
**Figure S241.**  $\sigma$ -profiles of 3-hexanone (CAS-RN: 589-38-8) obtained from screening charge distributions calculated at the BP-TZVP-COSMO level and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



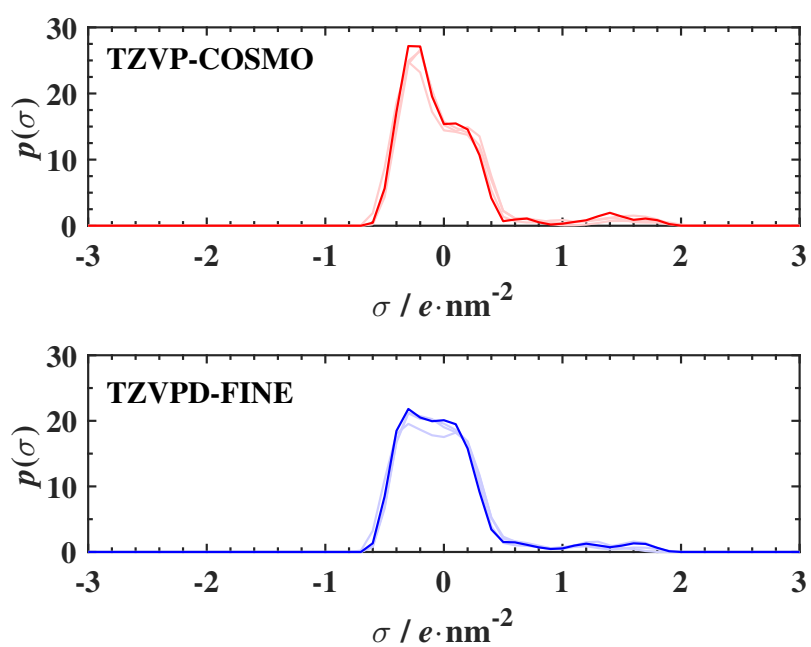
**Figure S242.**  $\sigma$ -profiles of cyclopentanone (CAS-RN: 120-92-3) obtained from screening charge distributions calculated at the BP-TZVP-COSMO level and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



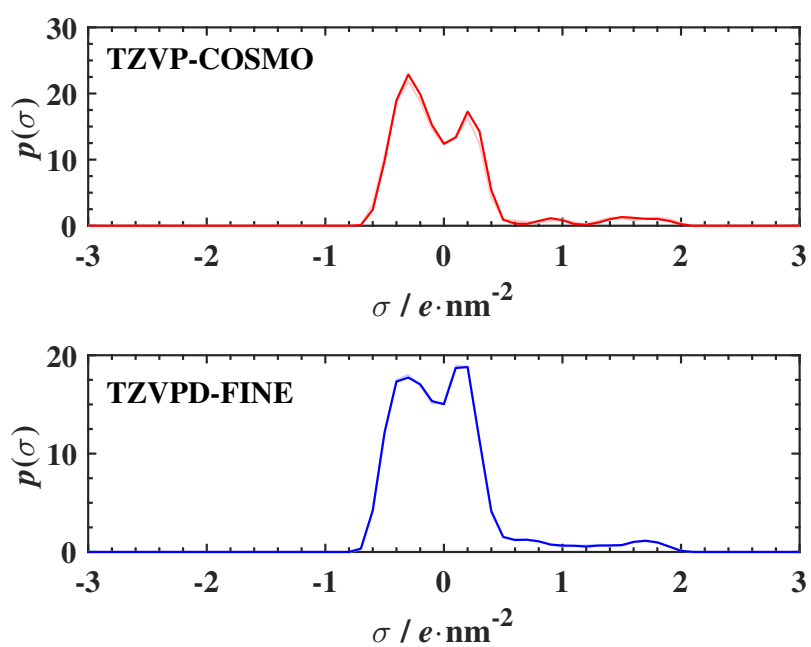
**Figure S243.**  $\sigma$ -profiles of cyclohexanone (CAS-RN: 108-94-1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO level and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



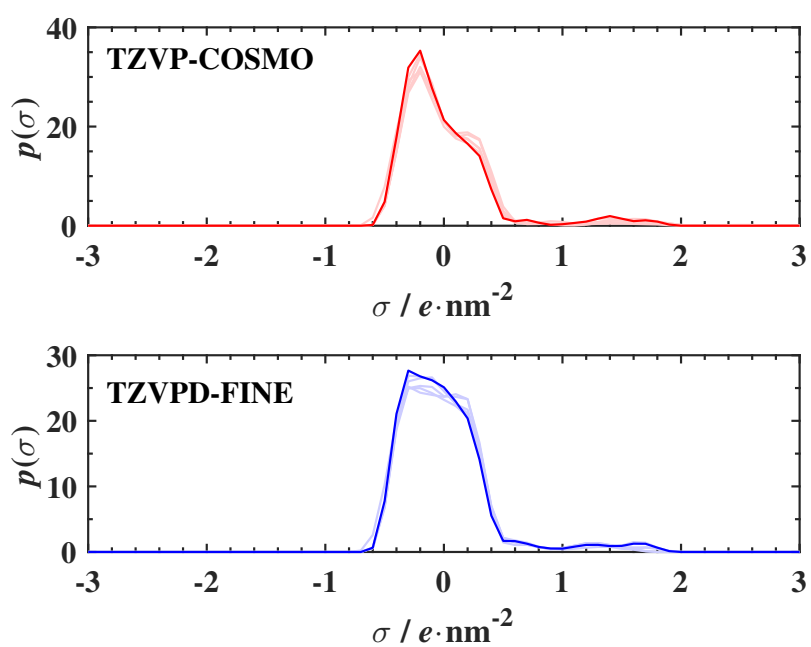
**Figure S244.**  $\sigma$ -profiles of diethyl ether (CAS-RN: 60-29-7) obtained from screening charge distributions calculated at the BP-TZVP-COSMO level and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



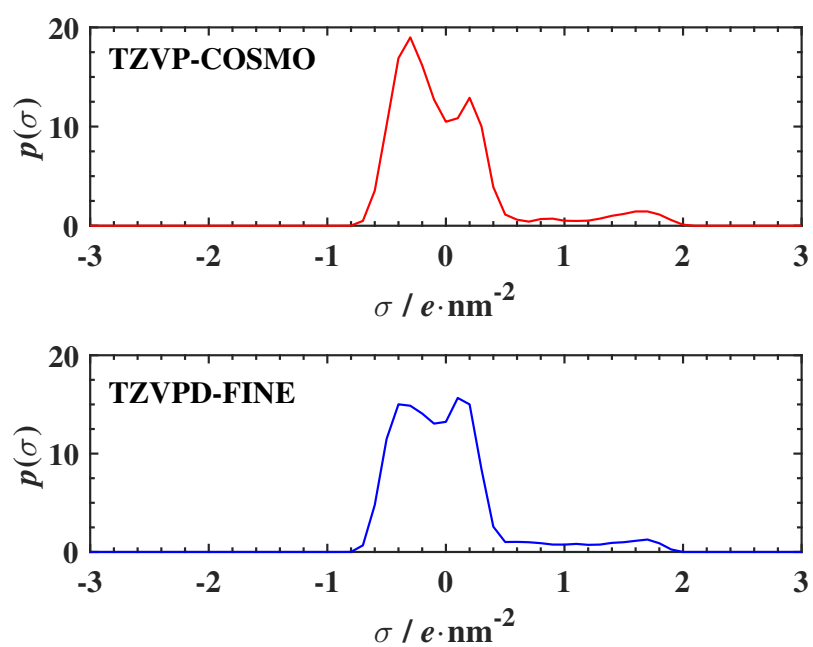
**Figure S245.**  $\sigma$ -profiles of di-*n*-propyl ether (CAS-RN: 111-43-3) obtained from screening charge distributions calculated at the BP-TZVP-COSMO level and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



**Figure S246.**  $\sigma$ -profiles of di-*iso*-propyl ether (CAS-RN: 108-20-3) obtained from screening charge distributions calculated at the BP-TZVP-COSMO level and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).

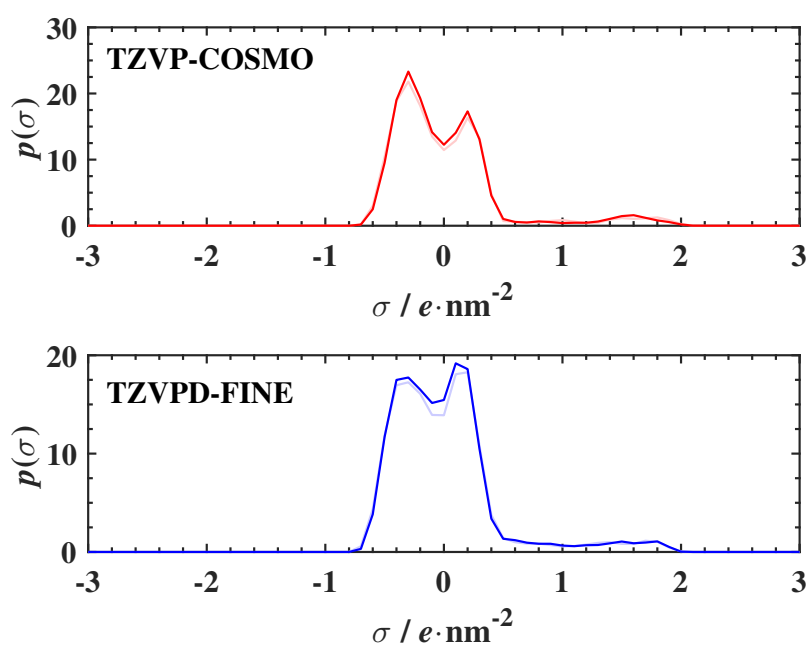


**Figure S247.**  $\sigma$ -profiles of di-*n*-butyl ether (CAS-RN: 142-96-1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO level and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).

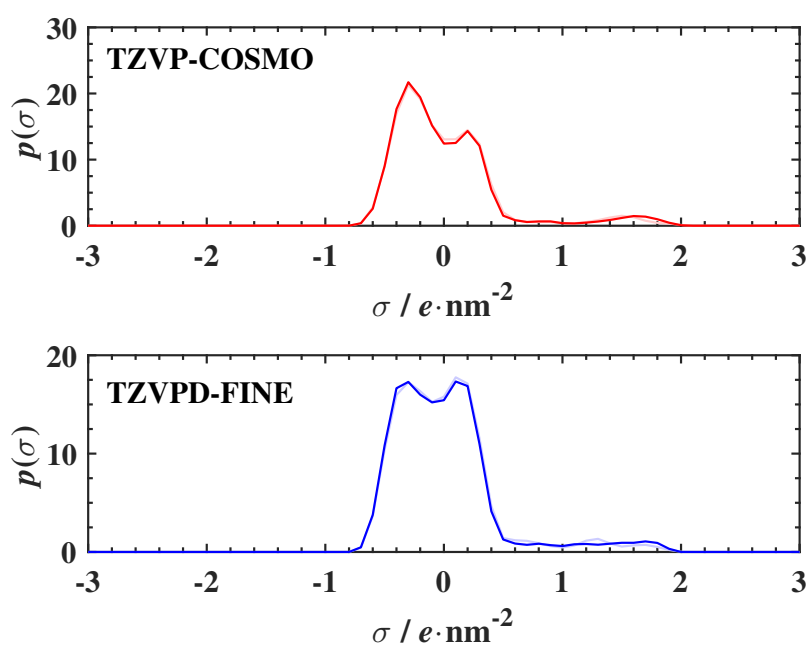


**Figure S248.**  $\sigma$ -profiles of *tert*-butylmethyl ether (CAS-RN: 1634-4-4) obtained from screening charge distributions calculated at the BP-TZVP-COSMO level and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).

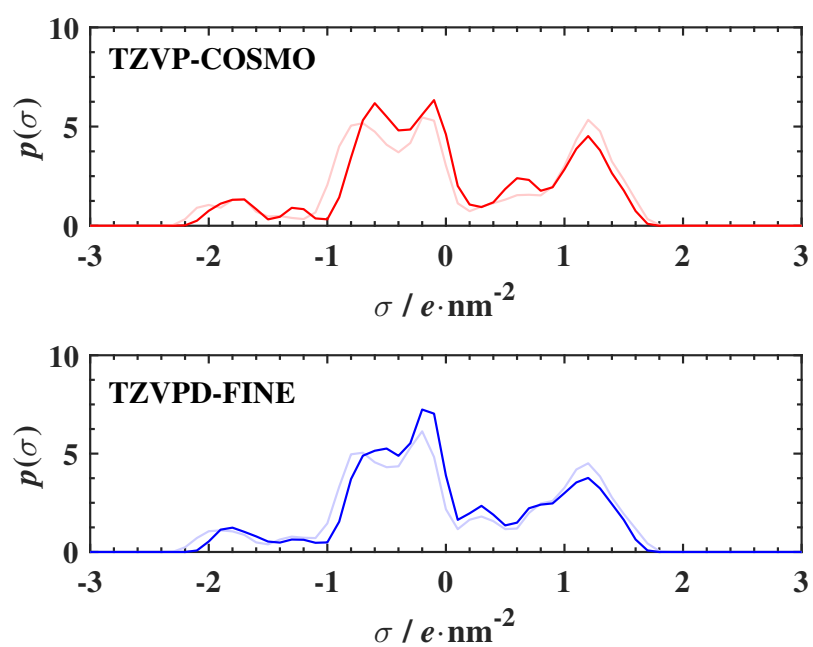




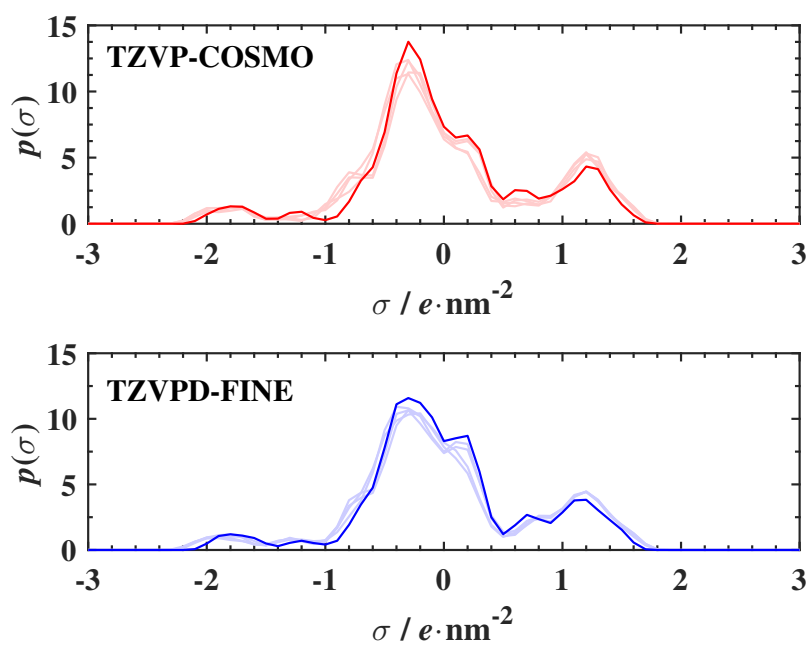
**Figure S249.**  $\sigma$ -profiles of *tert*-butylethyl ether (CAS-RN: 637-92-3) obtained from screening charge distributions calculated at the BP-TZVP-COSMO level and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



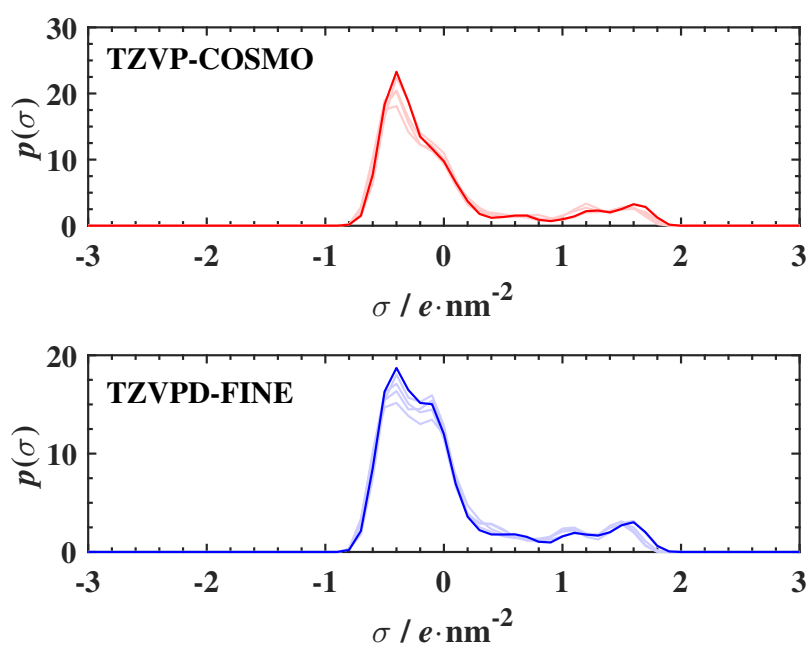
**Figure S250.**  $\sigma$ -profiles of *tert*-amylmethyl ether (CAS-RN: 994-5-8) obtained from screening charge distributions calculated at the BP-TZVP-COSMO level and BP-TZVPD-FINE levels. Thick lines are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



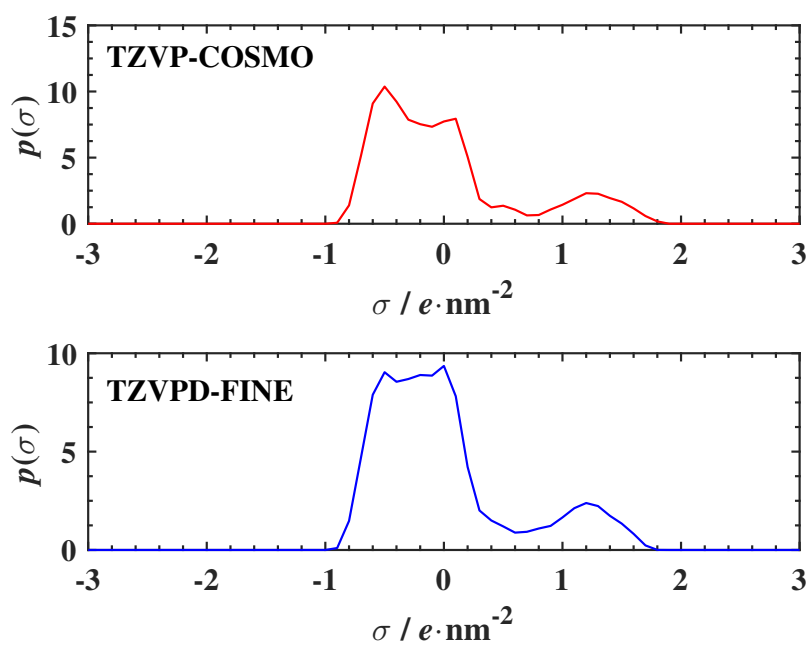
**Figure S251.**  $\sigma$ -profiles of acetic acid (CAS-RN: 64-19-7) obtained from screening charge distributions calculated at the BP-TZVP-COSMO level and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



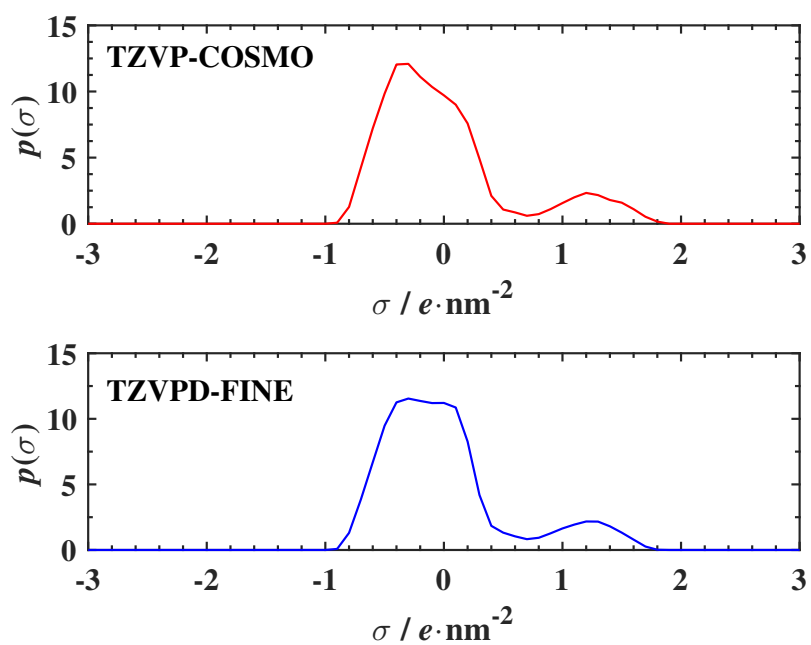
**Figure S252.**  $\sigma$ -profiles of butyric acid (CAS-RN: 107-92-6) obtained from screening charge distributions calculated at the BP-TZVP-COSMO level and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



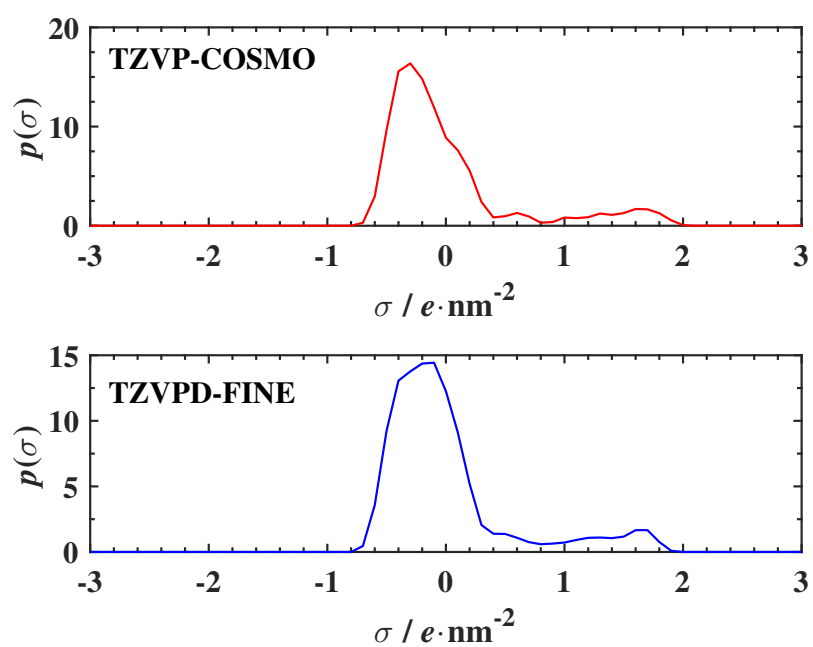
**Figure S253.**  $\sigma$ -profiles of 1,2-dimethoxyethane (CAS-RN: 110-71-4) obtained from screening charge distributions calculated at the BP-TZVP-COSMO level and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



**Figure S254.**  $\sigma$ -profiles of 1,2-epoxypropane (CAS-RN: 75-56-9) obtained from screening charge distributions calculated at the BP-TZVP-COSMO level and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).

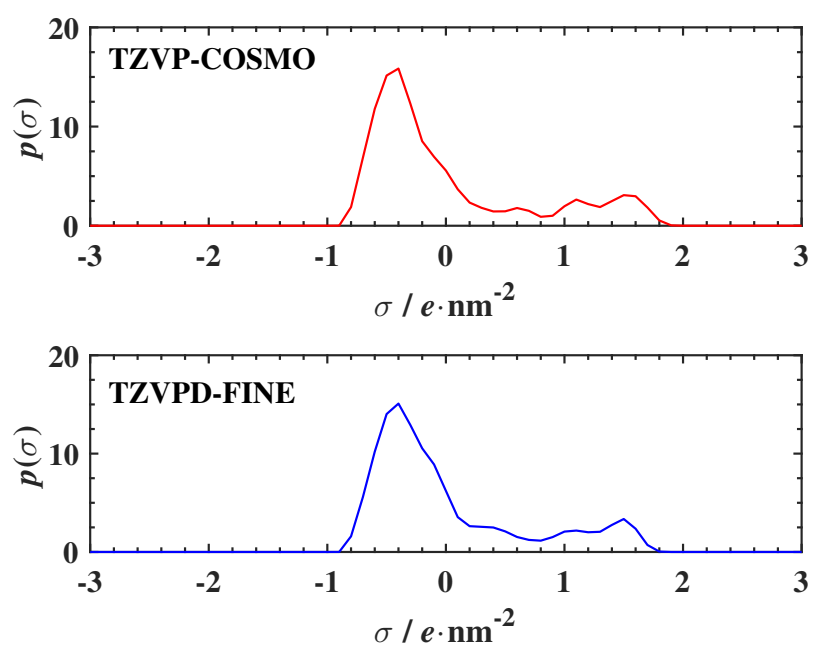


**Figure S255.**  $\sigma$ -profiles of 1,2-epoxybutane (CAS-RN: 106-88-7) obtained from screening charge distributions calculated at the BP-TZVP-COSMO level and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).

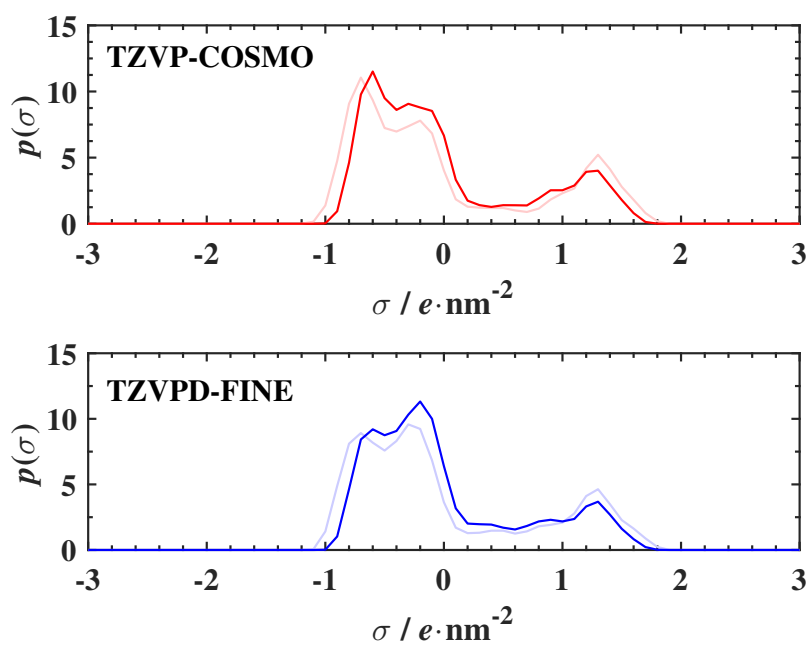


**Figure S256.**  $\sigma$ -profiles of tetrahydrofuran (CAS-RN: 109-99-9) obtained from screening charge distributions calculated at the BP-TZVP-COSMO level and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).

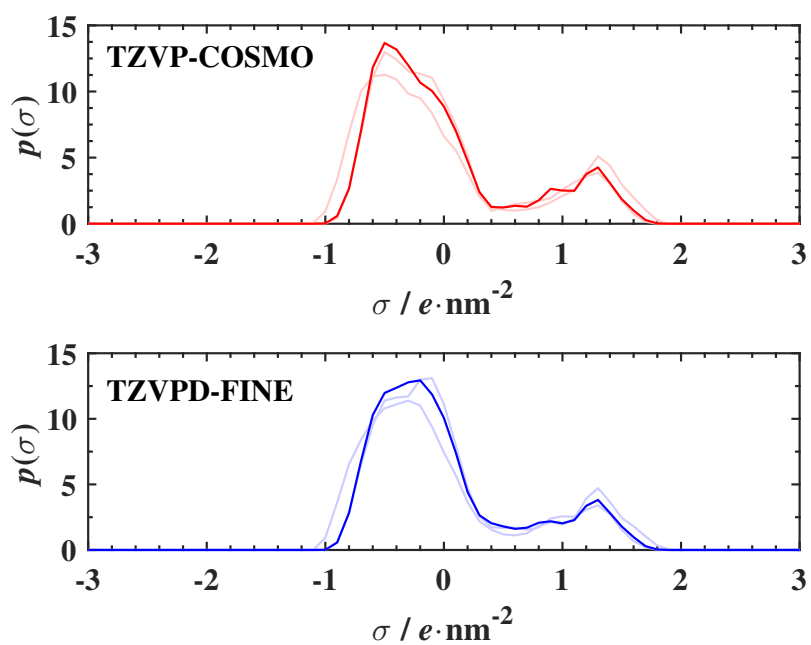




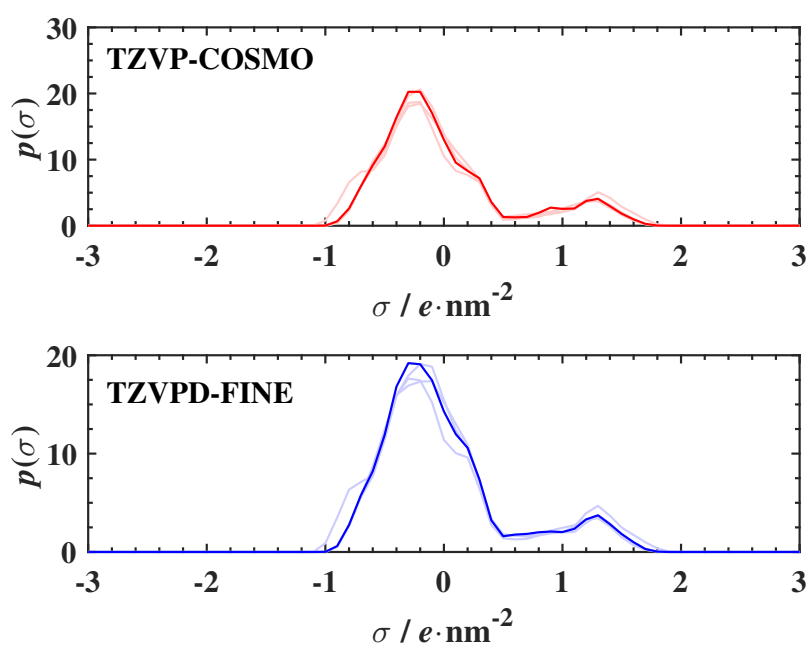
**Figure S257.**  $\sigma$ -profiles of 1,4-dioxane (CAS-RN: 123-91-1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO level and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



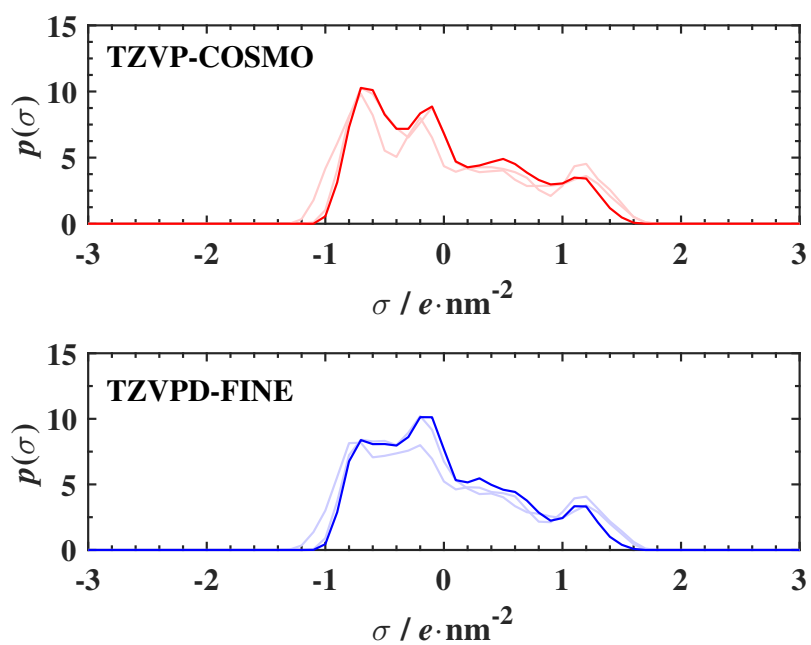
**Figure S258.**  $\sigma$ -profiles of methyl acetate (CAS-RN: 79-20-9) obtained from screening charge distributions calculated at the BP-TZVP-COSMO level and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



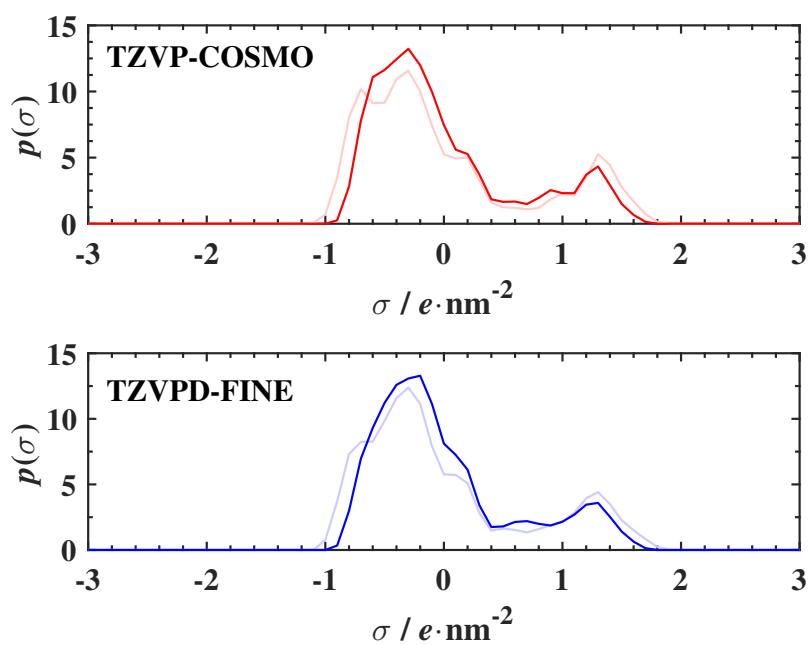
**Figure S259.**  $\sigma$ -profiles of ethyl acetate (CAS-RN: 141-78-6) obtained from screening charge distributions calculated at the BP-TZVP-COSMO level and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



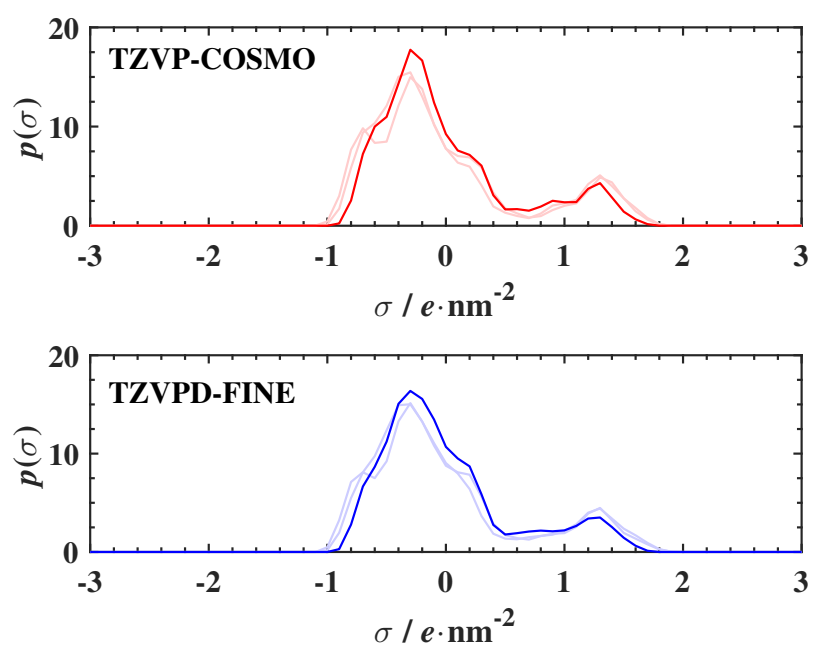
**Figure S260.**  $\sigma$ -profiles of butyl acetate (CAS-RN: 123-86-4) obtained from screening charge distributions calculated at the BP-TZVP-COSMO level and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



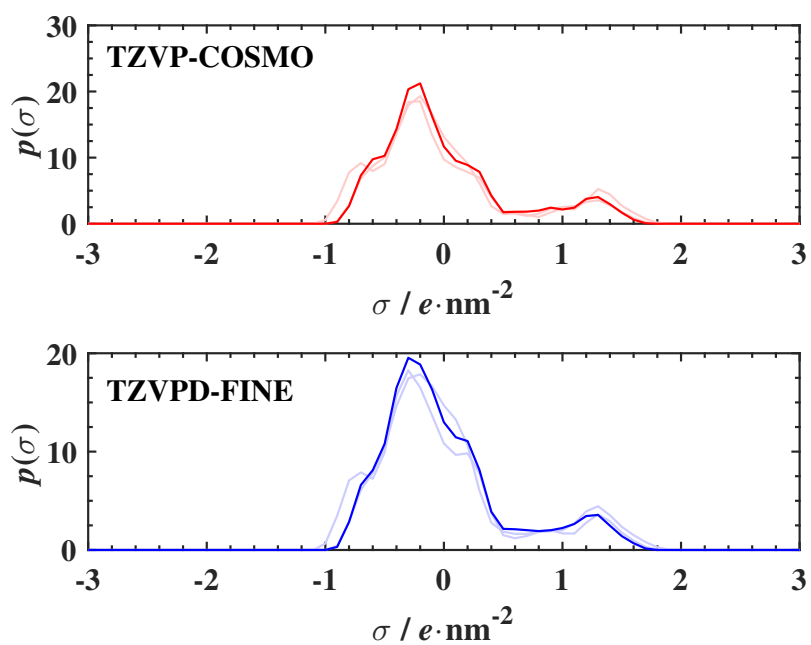
**Figure S261.**  $\sigma$ -profiles of vinyl acetate (CAS-RN: 108-5-4) obtained from screening charge distributions calculated at the BP-TZVP-COSMO level and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



**Figure S262.**  $\sigma$ -profiles of methyl propanoate (CAS-RN: 554-12-1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO level and BP-TZVPD-FINE levels. Thick lines are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).

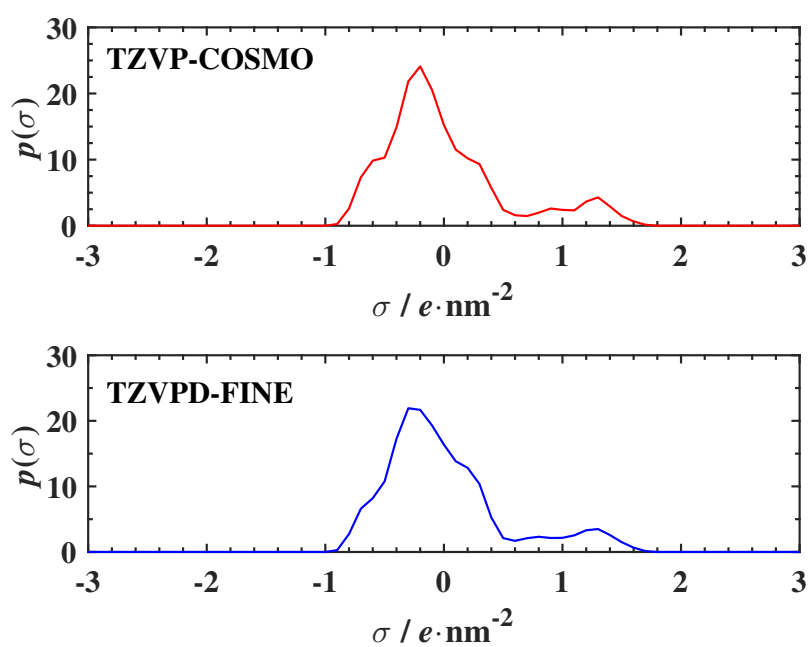


**Figure S263.**  $\sigma$ -profiles of methyl butanoate (CAS-RN: 623-42-7) obtained from screening charge distributions calculated at the BP-TZVP-COSMO level and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).

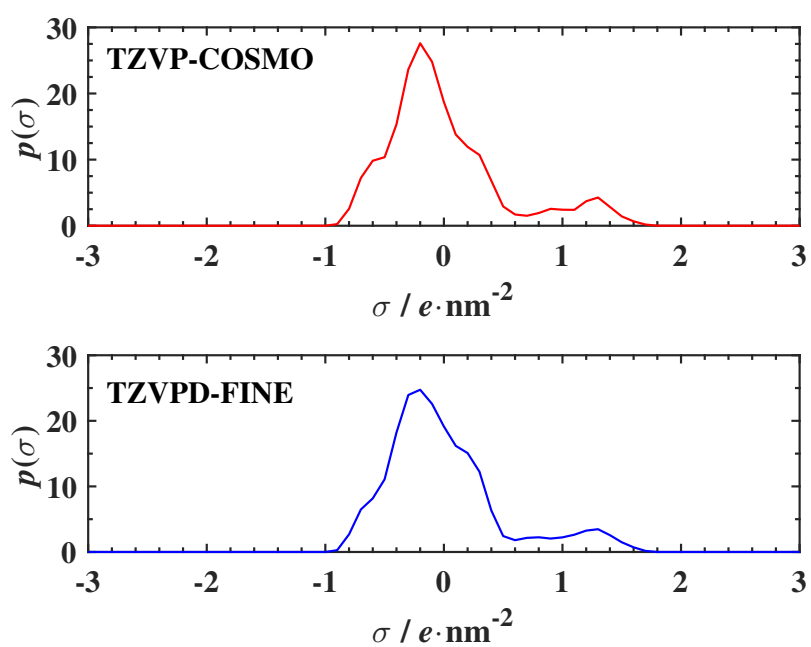


**Figure S264.**  $\sigma$ -profiles of methyl pentanoate (CAS-RN: 624-24-8) obtained from screening charge distributions calculated at the BP-TZVP-COSMO level and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).

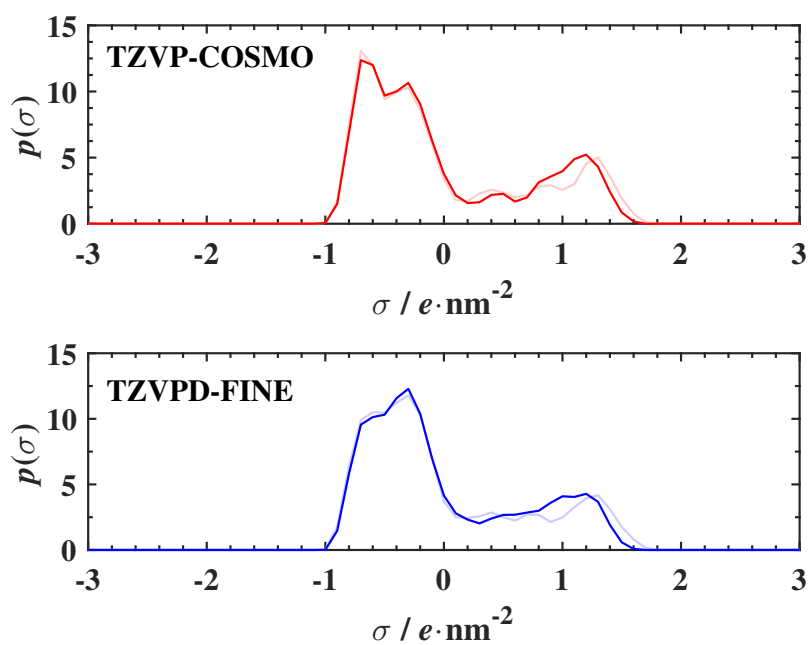




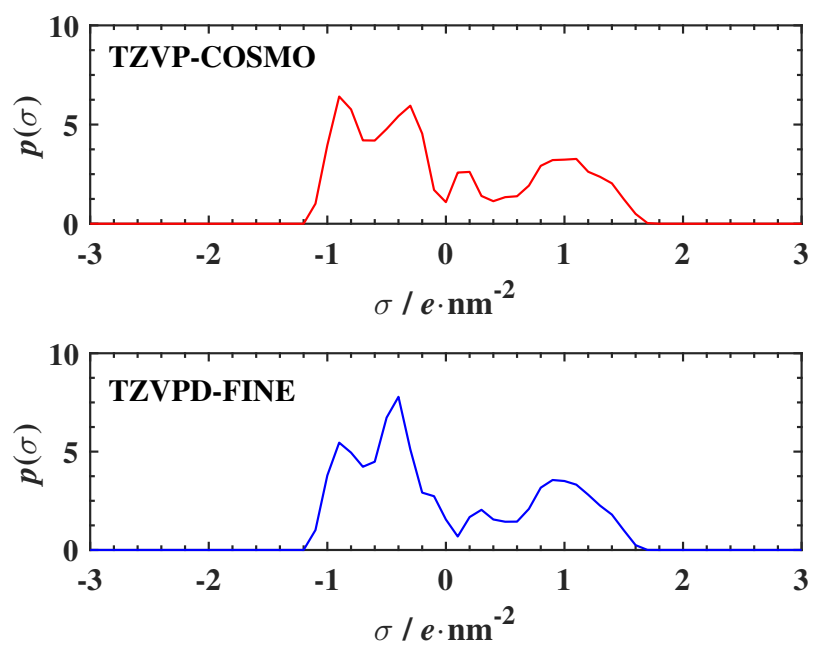
**Figure S265.**  $\sigma$ -profiles of methyl hexanoate (CAS-RN: 106-70-7) obtained from screening charge distributions calculated at the BP-TZVP-COSMO level and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



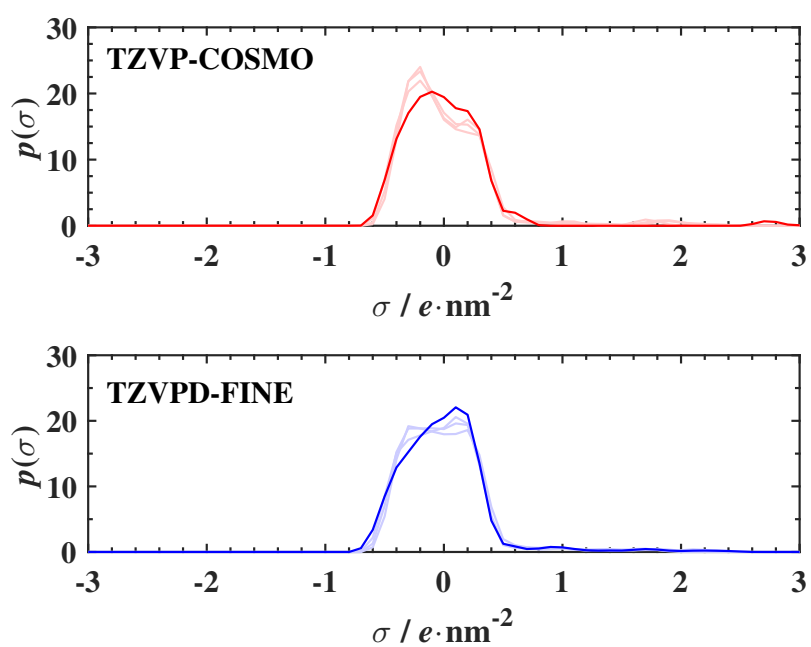
**Figure S266.**  $\sigma$ -profiles of methyl heptanoate (CAS-RN: 106-73-0) obtained from screening charge distributions calculated at the BP-TZVP-COSMO level and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



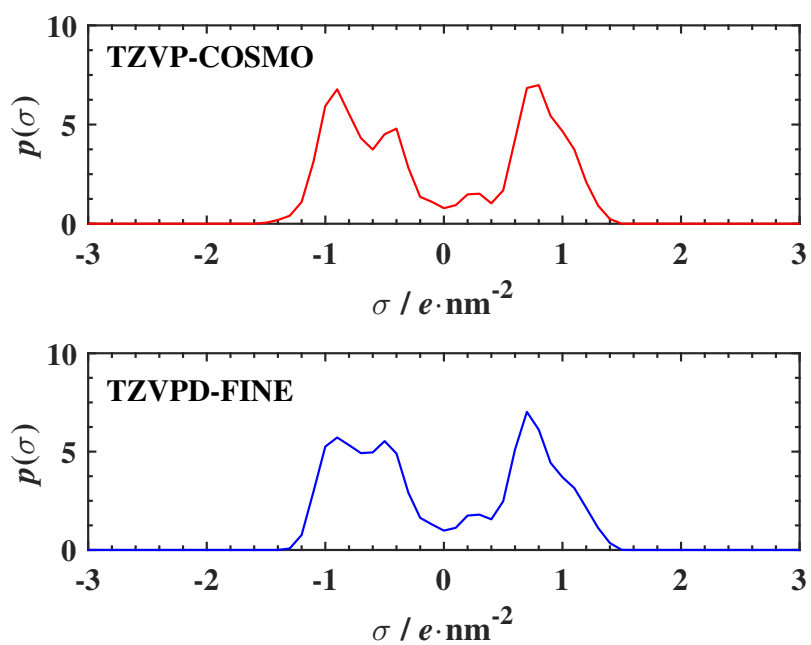
**Figure S267.**  $\sigma$ -profiles of dimethyl carbonate (CAS-RN: 616-38-6) obtained from screening charge distributions calculated at the BP-TZVP-COSMO level and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



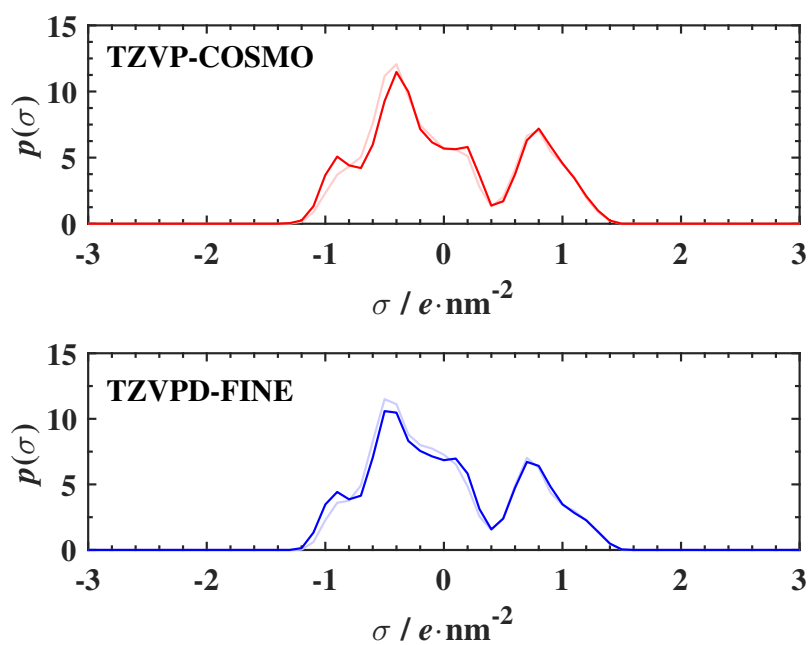
**Figure S268.**  $\sigma$ -profiles of acetonitrile (CAS-RN: 75-5-8) obtained from screening charge distributions calculated at the BP-TZVP-COSMO level and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



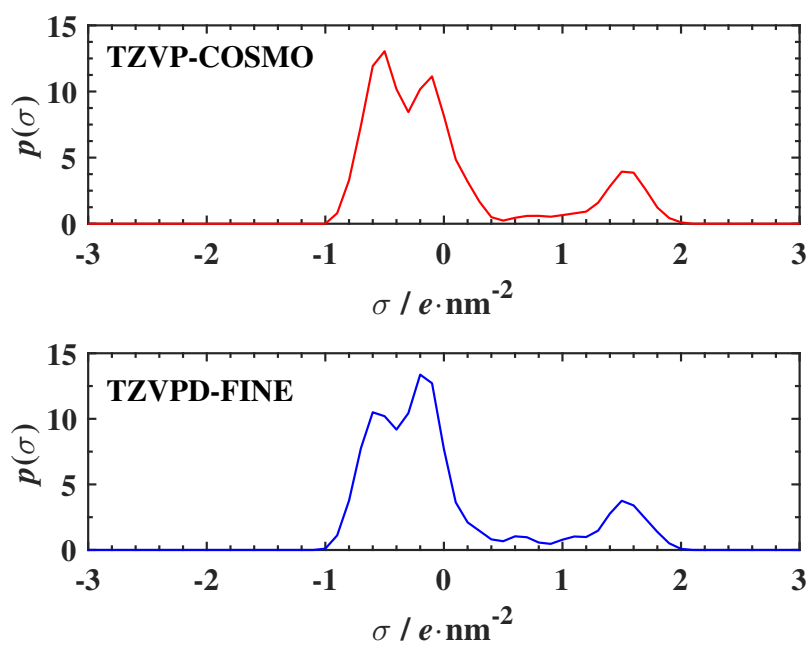
**Figure S269.**  $\sigma$ -profiles of triethylamine (CAS-RN: 121-44-8) obtained from screening charge distributions calculated at the BP-TZVP-COSMO level and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



**Figure S270.**  $\sigma$ -profiles of nitromethane (CAS-RN: 75-52-5) obtained from screening charge distributions calculated at the BP-TZVP-COSMO level and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).

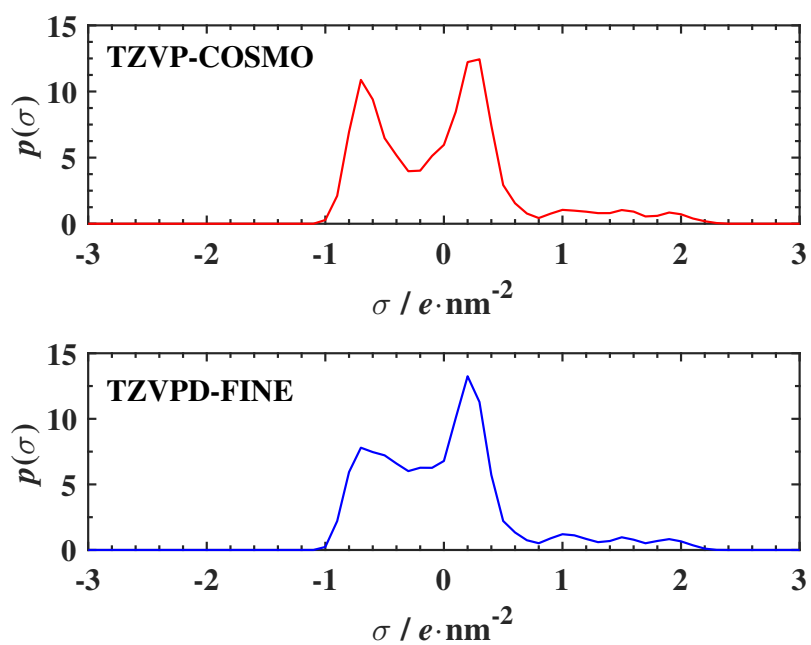


**Figure S271.**  $\sigma$ -profiles of 1-nitropropane (CAS-RN: 108-3-2) obtained from screening charge distributions calculated at the BP-TZVP-COSMO level and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).

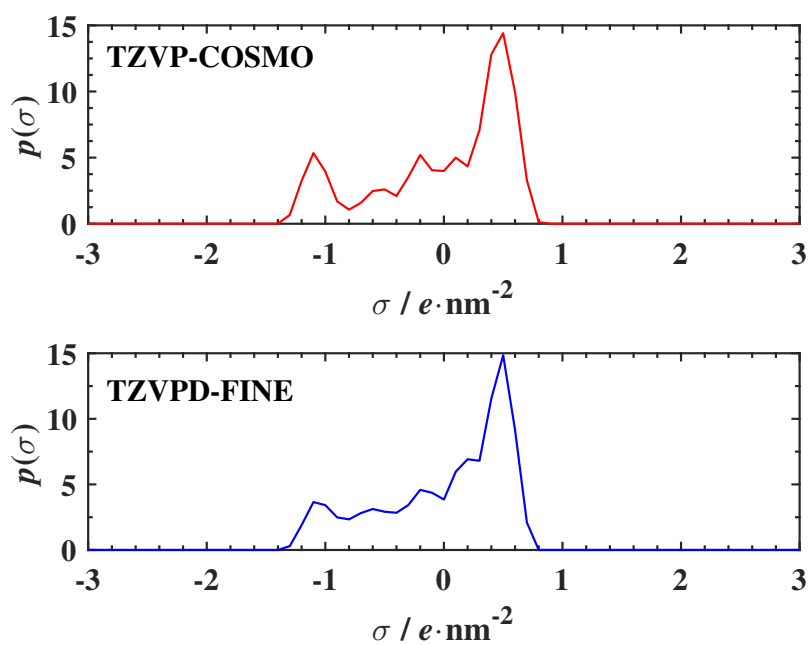


**Figure S272.**  $\sigma$ -profiles of *N,N*-dimethylformamide (CAS-RN: 68-12-2) obtained from screening charge distributions calculated at the BP-TZVP-COSMO level and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).

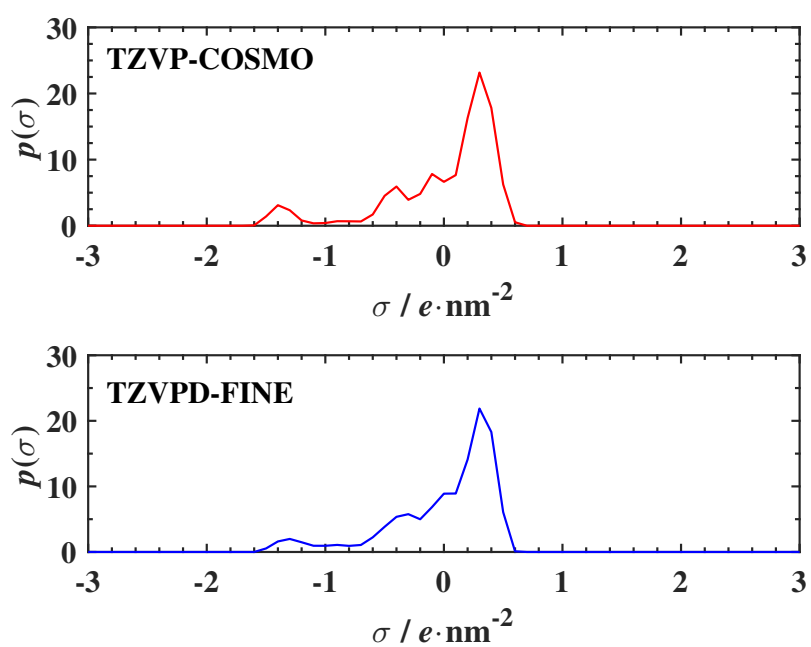




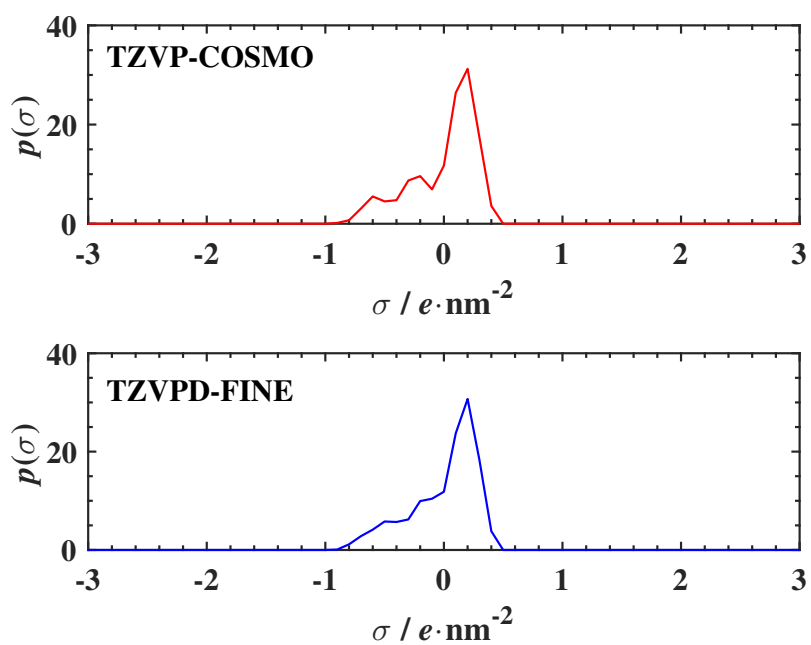
**Figure S273.**  $\sigma$ -profiles of pyridine (CAS-RN: 110-86-1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO level and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



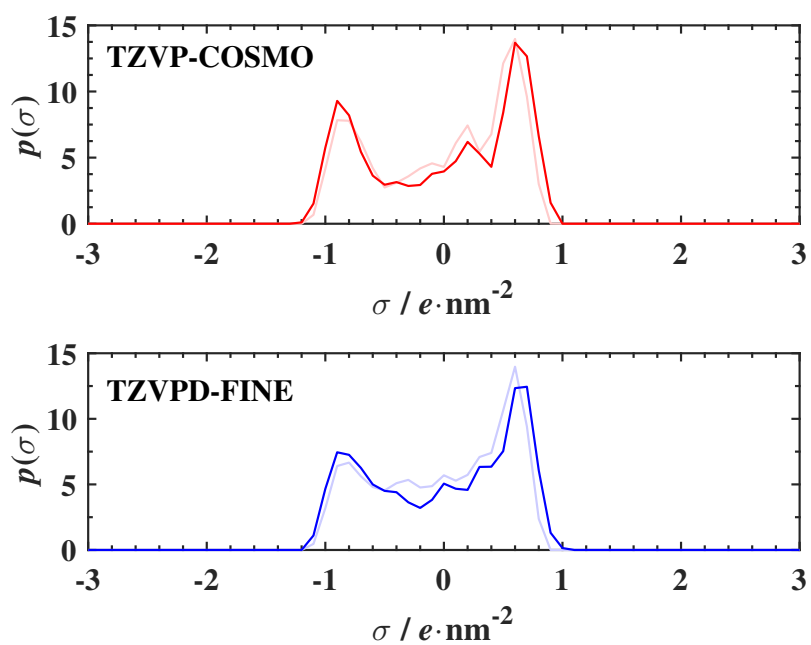
**Figure S274.**  $\sigma$ -profiles of dichloromethane (CAS-RN: 75-9-2) obtained from screening charge distributions calculated at the BP-TZVP-COSMO level and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



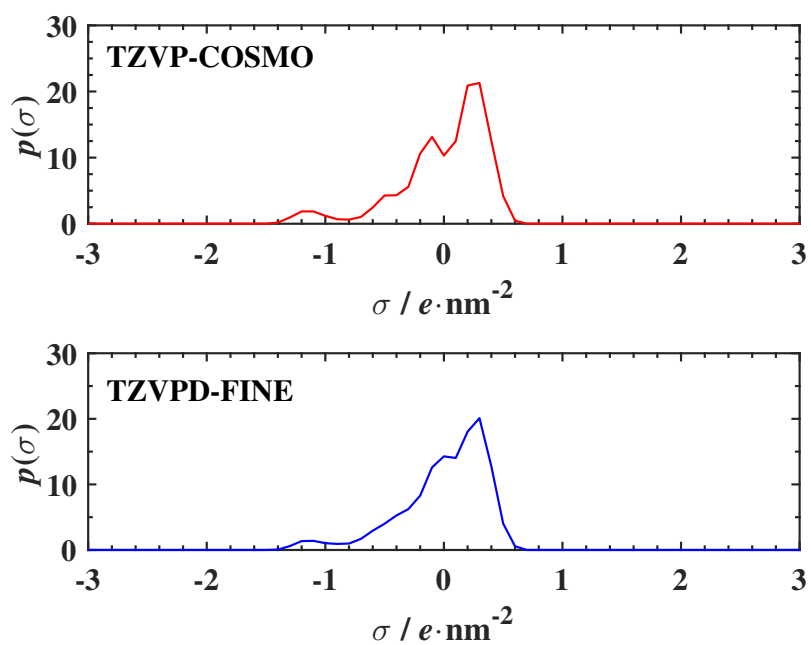
**Figure S275.**  $\sigma$ -profiles of trichloromethane (CAS-RN: 67-66-3) obtained from screening charge distributions calculated at the BP-TZVP-COSMO level and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



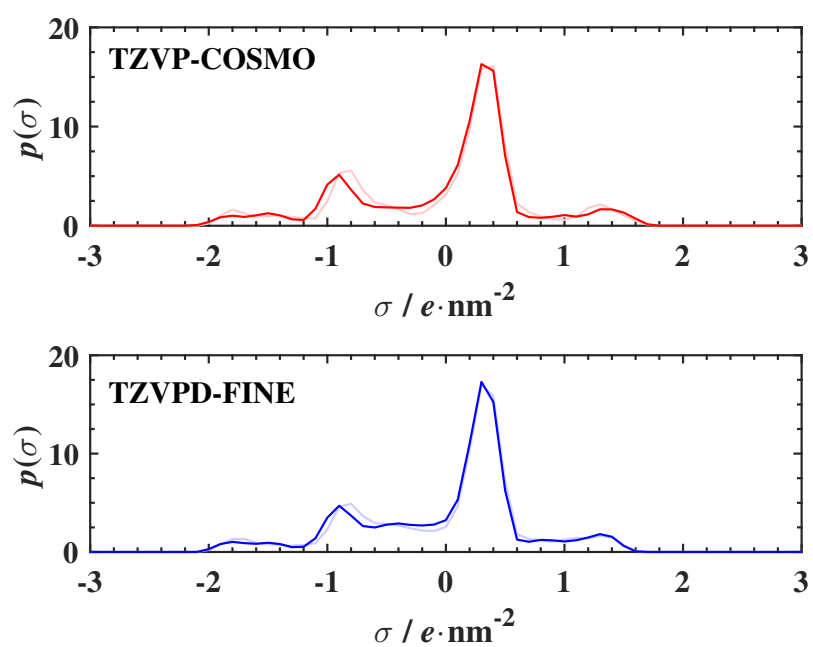
**Figure S276.**  $\sigma$ -profiles of tetrachloromethane (CAS-RN: 56-23-5) obtained from screening charge distributions calculated at the BP-TZVP-COSMO level and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



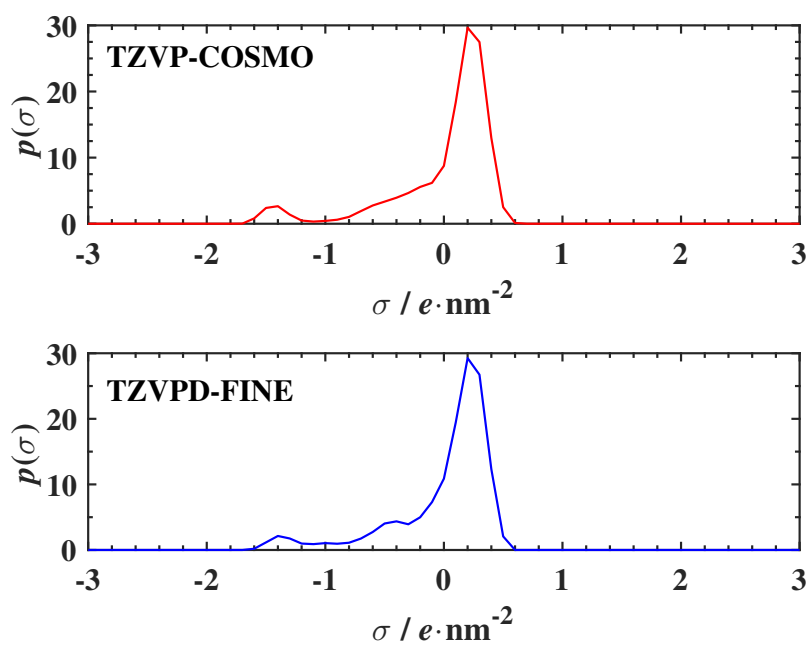
**Figure S277.**  $\sigma$ -profiles of 1,2-dichloroethane (CAS-RN: 107-6-2) obtained from screening charge distributions calculated at the BP-TZVP-COSMO level and BP-TZVPD-FINE levels. Thick lines are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



**Figure S278.**  $\sigma$ -profiles of trichloroethylene (CAS-RN: 79-1-6) obtained from screening charge distributions calculated at the BP-TZVP-COSMO level and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).

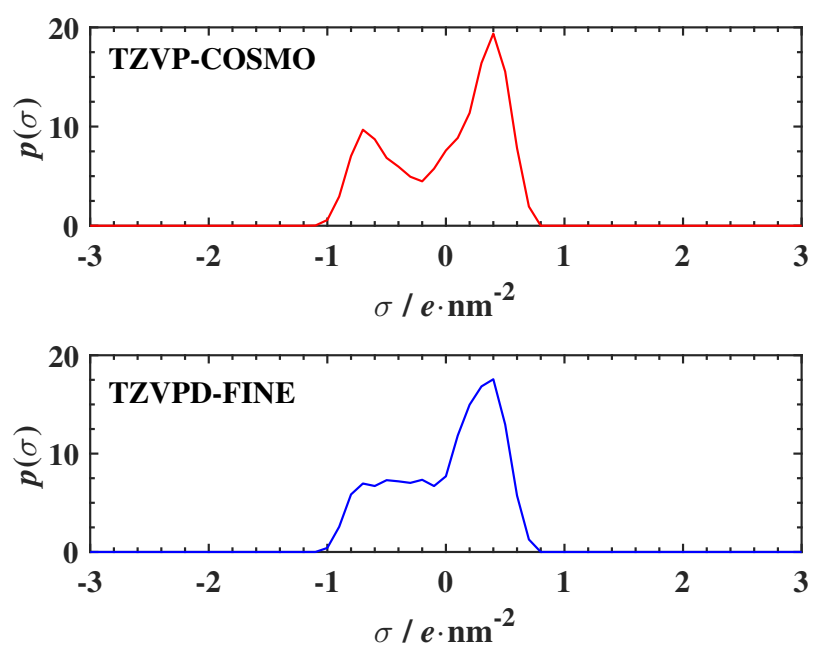


**Figure S279.**  $\sigma$ -profiles of 2,2,2-trifluoroethanol (CAS-RN: 75-89-8) obtained from screening charge distributions calculated at the BP-TZVP-COSMO level and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).

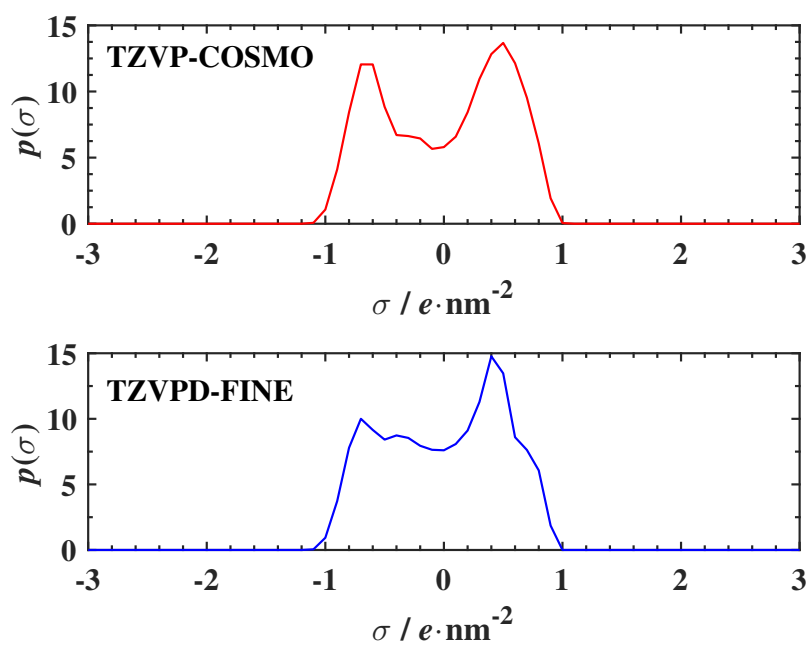


**Figure S280.**  $\sigma$ -profiles of halothane (CAS-RN: 151-67-7) obtained from screening charge distributions calculated at the BP-TZVP-COSMO level and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).

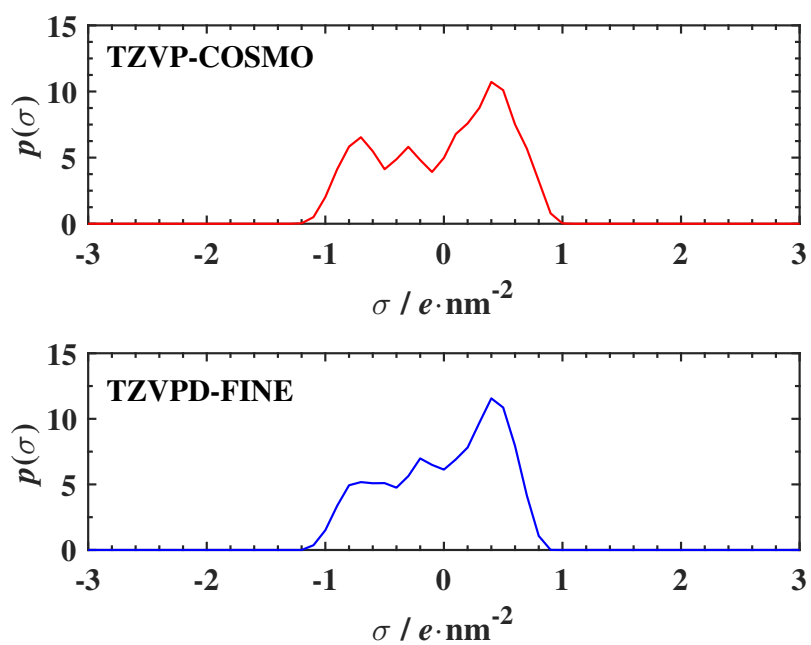




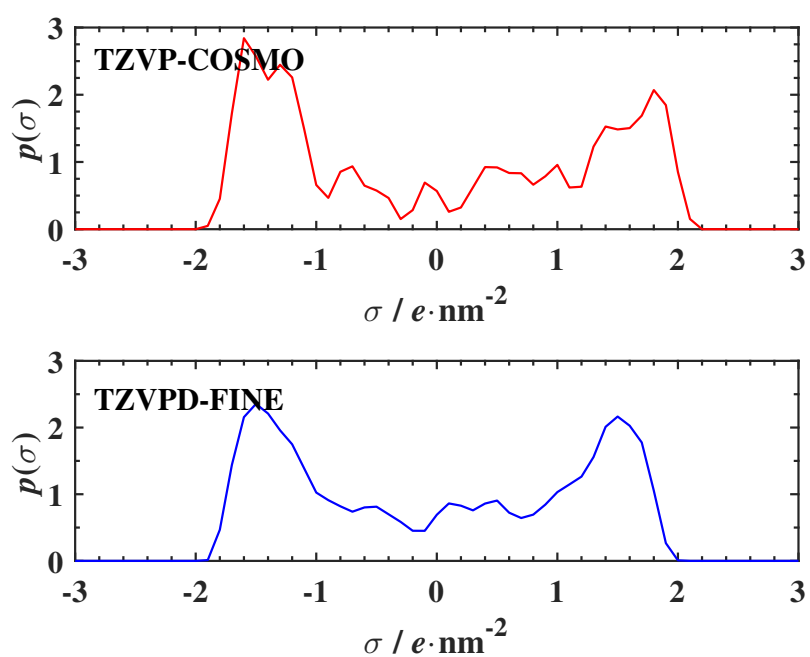
**Figure S281.**  $\sigma$ -profiles of bromobenzene (CAS-RN: 108-86-1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO level and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



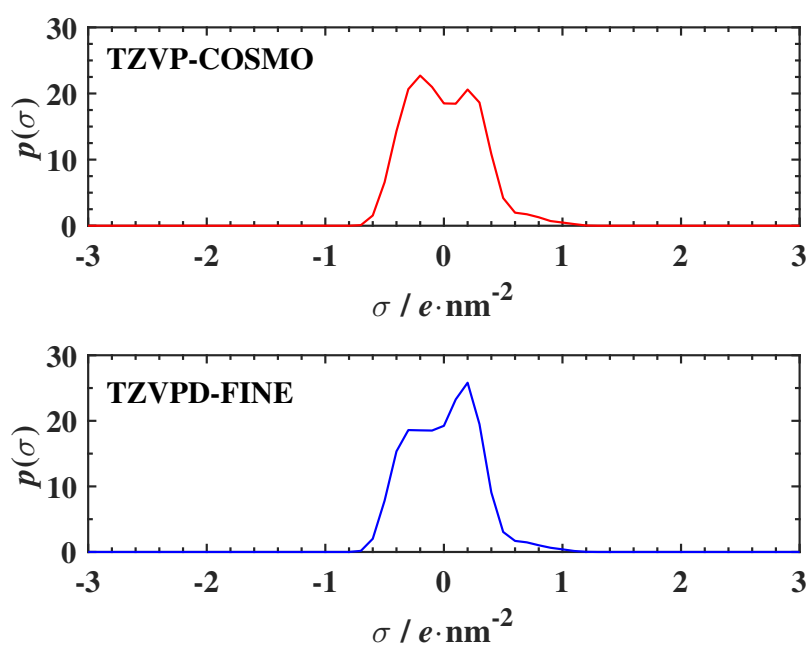
**Figure S282.**  $\sigma$ -profiles of chlorobenzene (CAS-RN: 100-44-7) obtained from screening charge distributions calculated at the BP-TZVP-COSMO level and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



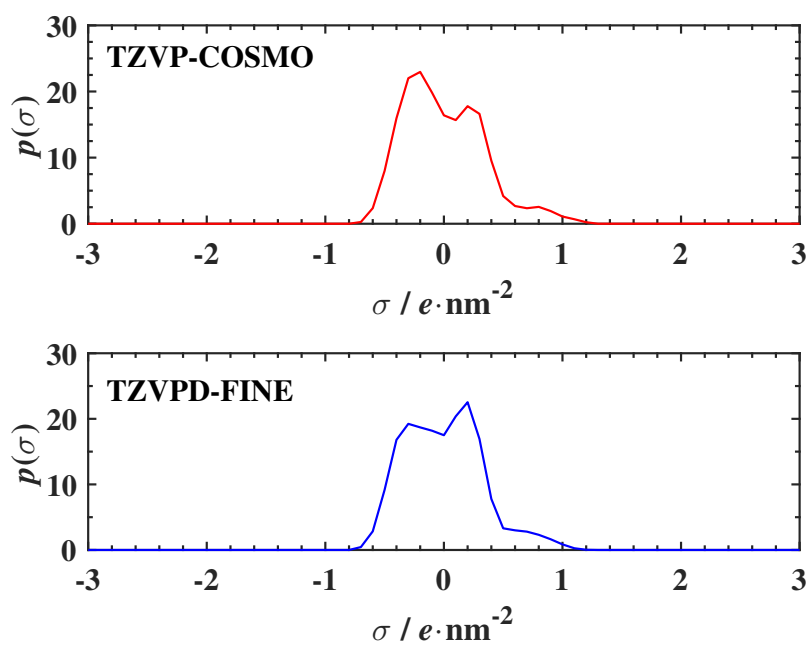
**Figure S283.**  $\sigma$ -profiles of thiophene (CAS-RN: 110-2-1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO level and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



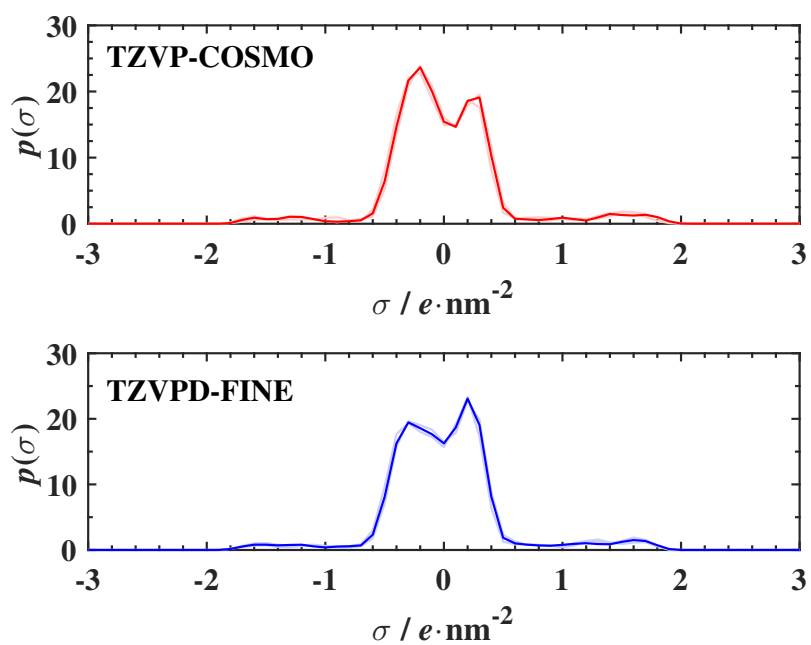
**Figure S284.**  $\sigma$ -profiles of water (CAS-RN: 7732-18-5) obtained from screening charge distributions calculated at the BP-TZVP-COSMO level and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



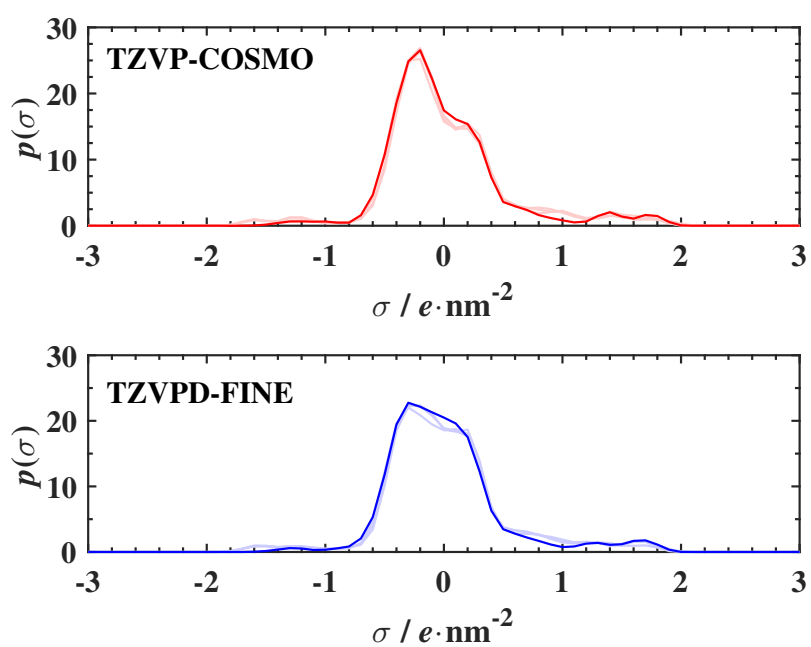
**Figure S285.**  $\sigma$ -profiles of  $\alpha$ -pinene (CAS-RN: 80-56-8) obtained from screening charge distributions calculated at the BP-TZVP-COSMO level and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



**Figure S286.**  $\sigma$ -profiles of  $\beta$ -pinene (CAS-RN: 18172-67-3) obtained from screening charge distributions calculated at the BP-TZVP-COSMO level and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).

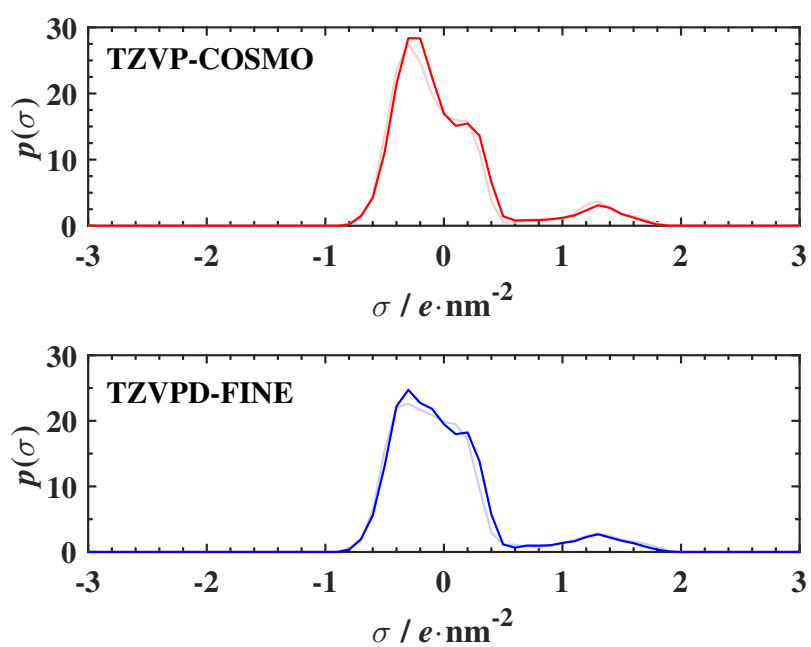


**Figure S287.**  $\sigma$ -profiles of (-)-borneol (CAS-RN: 464-45-9) obtained from screening charge distributions calculated at the BP-TZVP-COSMO level and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).

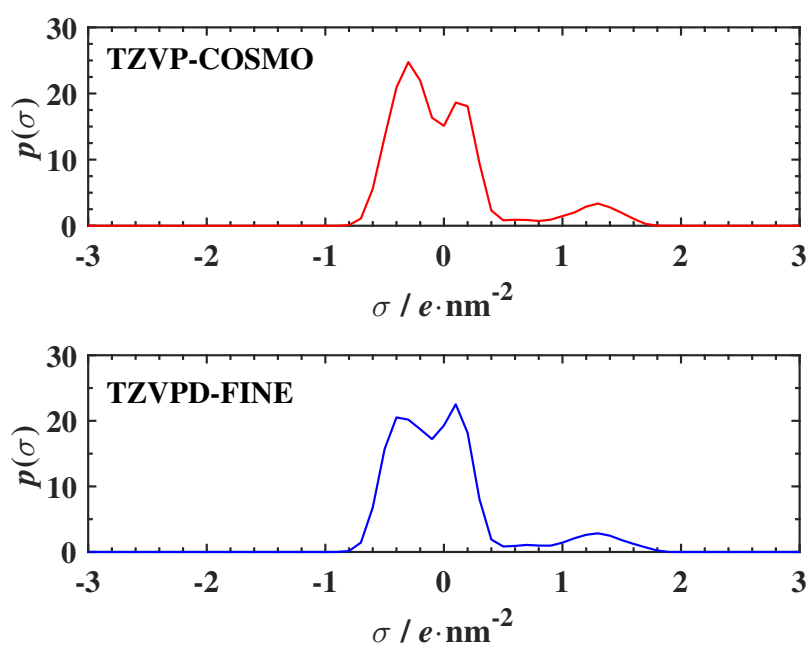


**Figure S288.**  $\sigma$ -profiles of (-)-isopulegol (CAS-RN: 89-79-2) obtained from screening charge distributions calculated at the BP-TZVP-COSMO level and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).

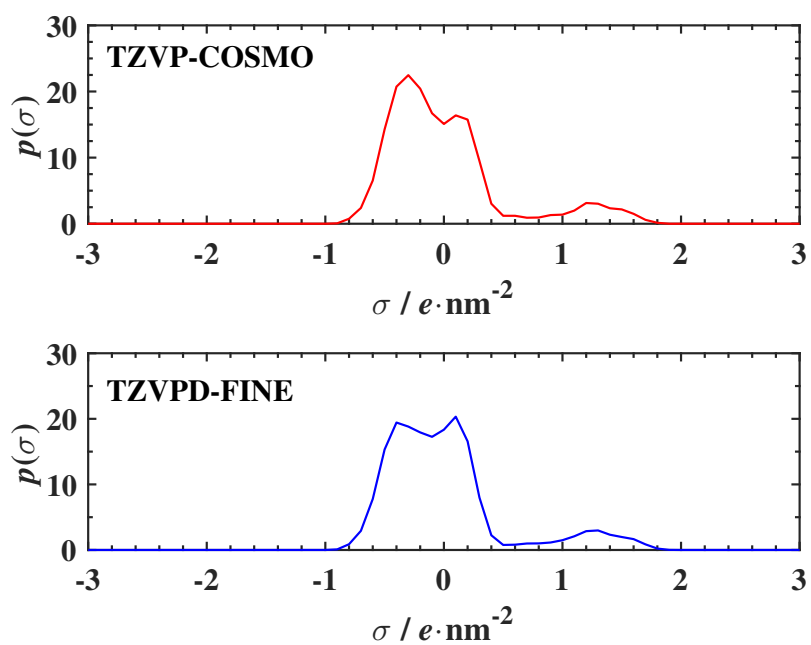




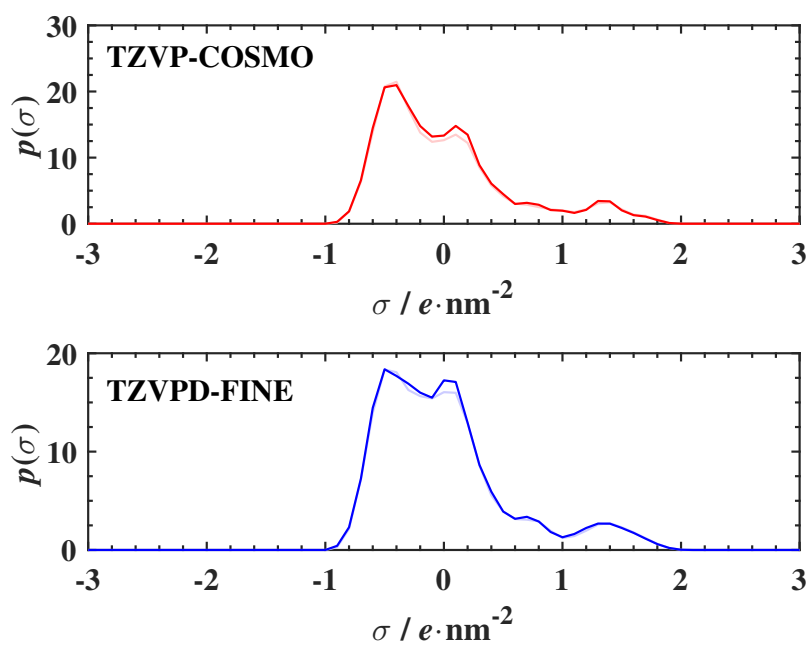
**Figure S289.**  $\sigma$ -profiles of (-)-menthone (CAS-RN: 14073-97-3) obtained from screening charge distributions calculated at the BP-TZVP-COSMO level and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



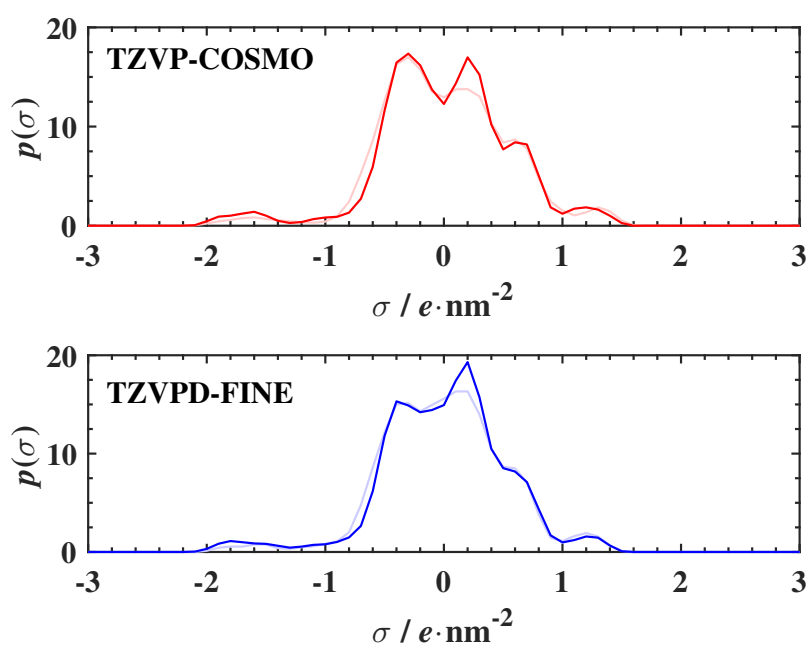
**Figure S290.**  $\sigma$ -profiles of (1R)-(-)-fenchone (CAS-RN: 7787-20-4) obtained from screening charge distributions calculated at the BP-TZVP-COSMO level and BP-TZVPD-FINE levels. Thick lines are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



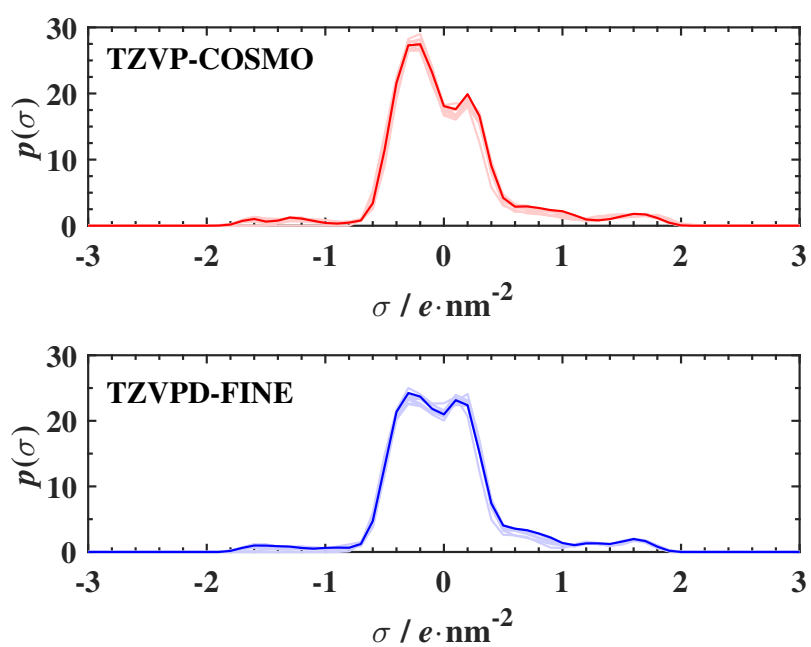
**Figure S291.**  $\sigma$ -profiles of (*R*)-(+)-camphor (CAS-RN: 464-49-3) obtained from screening charge distributions calculated at the BP-TZVP-COSMO level and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



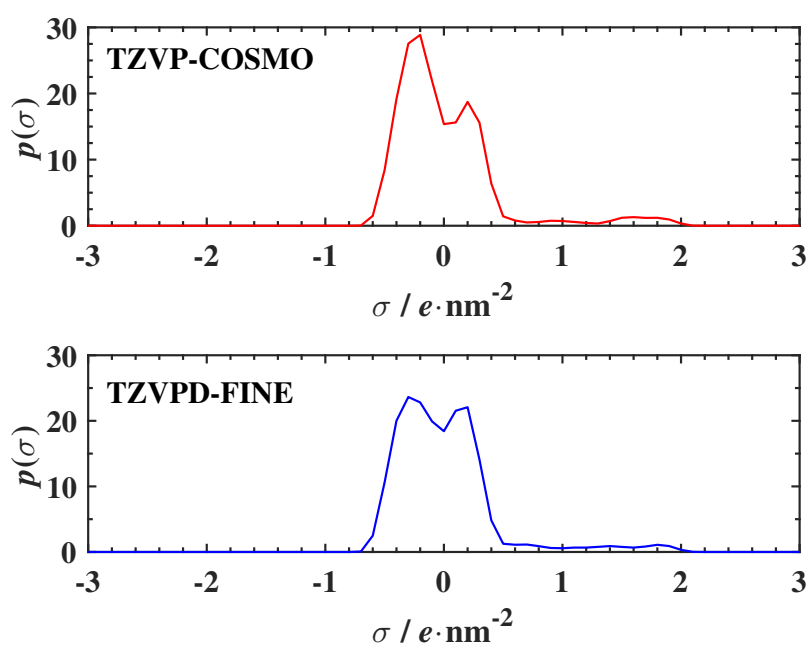
**Figure S292.**  $\sigma$ -profiles of (*S*)-(+)-carvone (CAS-RN: 2244-16-8) obtained from screening charge distributions calculated at the BP-TZVP-COSMO level and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



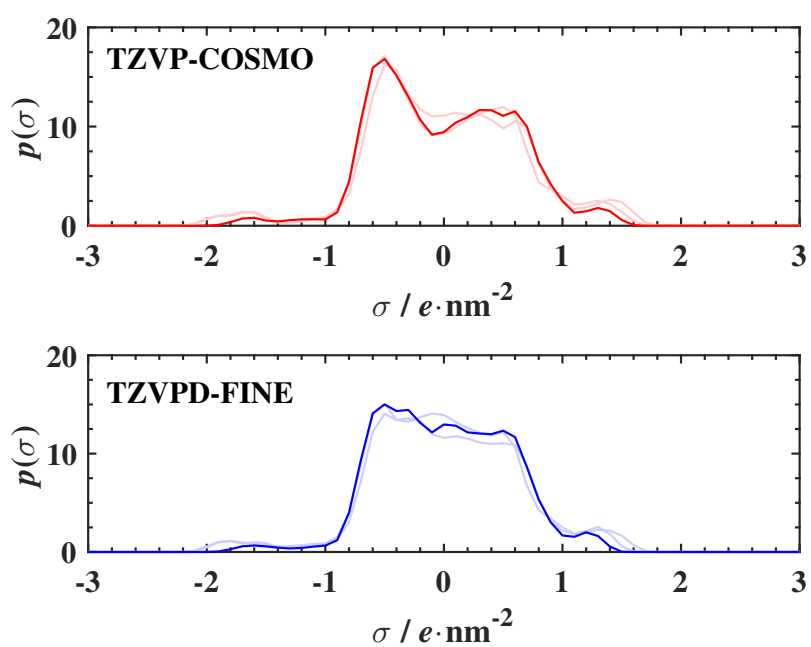
**Figure S293.**  $\sigma$ -profiles of carvacrol (CAS-RN: 499-75-2) obtained from screening charge distributions calculated at the BP-TZVP-COSMO level and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



**Figure S294.**  $\sigma$ -profiles of DL-citronellol (CAS-RN: 106-22-9) obtained from screening charge distributions calculated at the BP-TZVP-COSMO level and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).

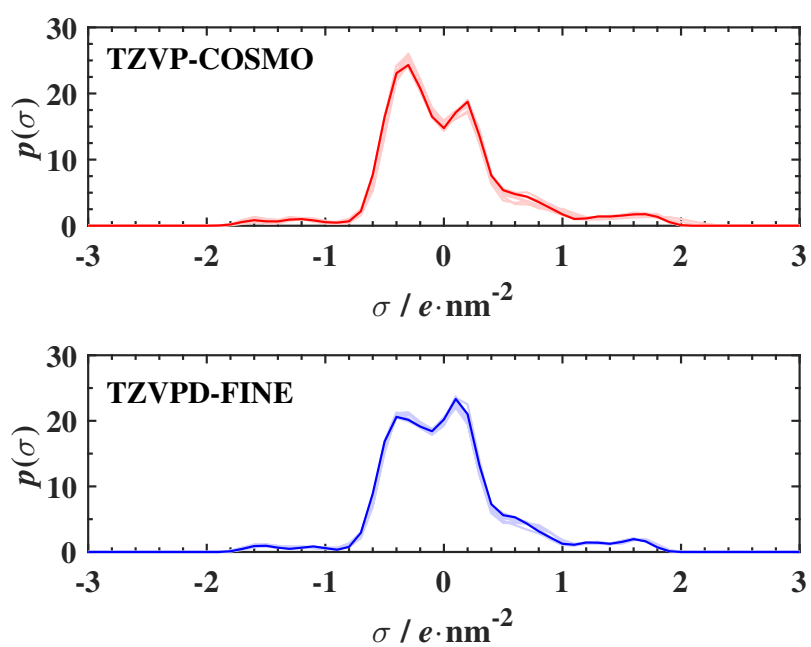


**Figure S295.**  $\sigma$ -profiles of eucalyptol (CAS-RN: 470-82-6) obtained from screening charge distributions calculated at the BP-TZVP-COSMO level and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).

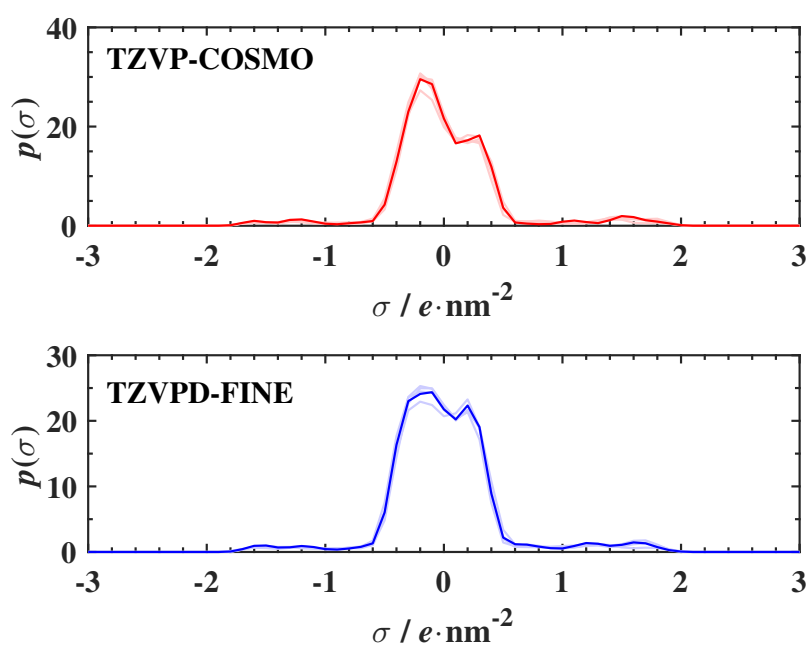


**Figure S296.**  $\sigma$ -profiles of eugenol (CAS-RN: 97-53-0) obtained from screening charge distributions calculated at the BP-TZVP-COSMO level and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).

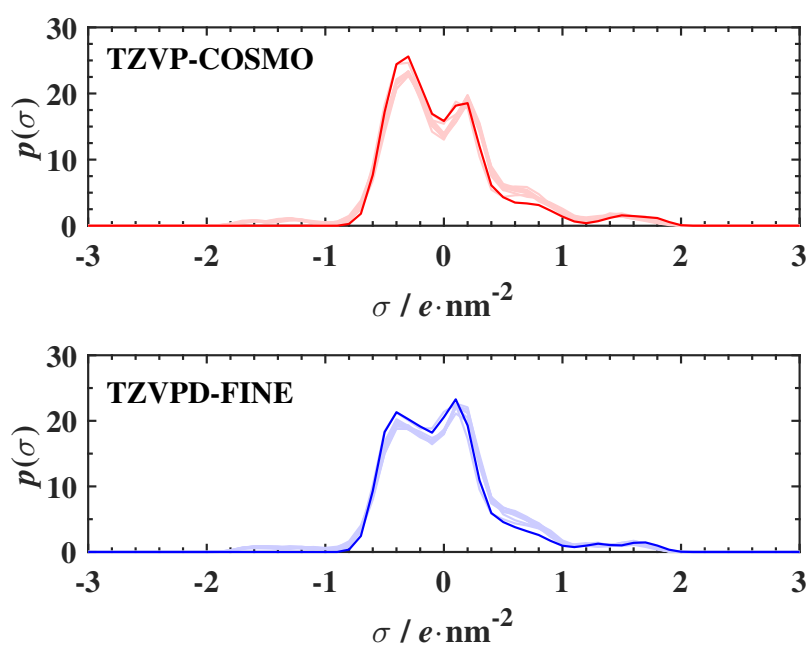




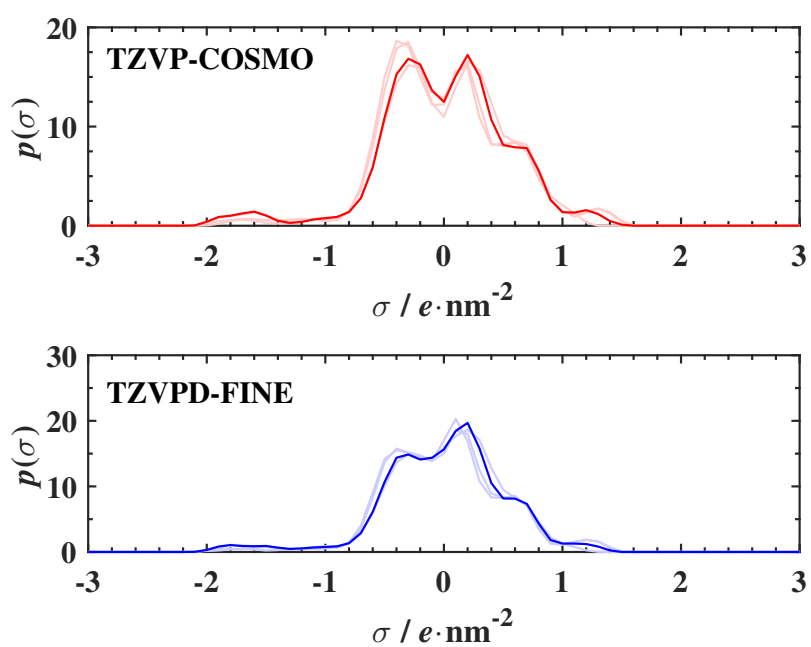
**Figure S297.**  $\sigma$ -profiles of geraniol (CAS-RN: 106-24-1) obtained from screening charge distributions calculated at the BP-TZVP-COSMO level and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



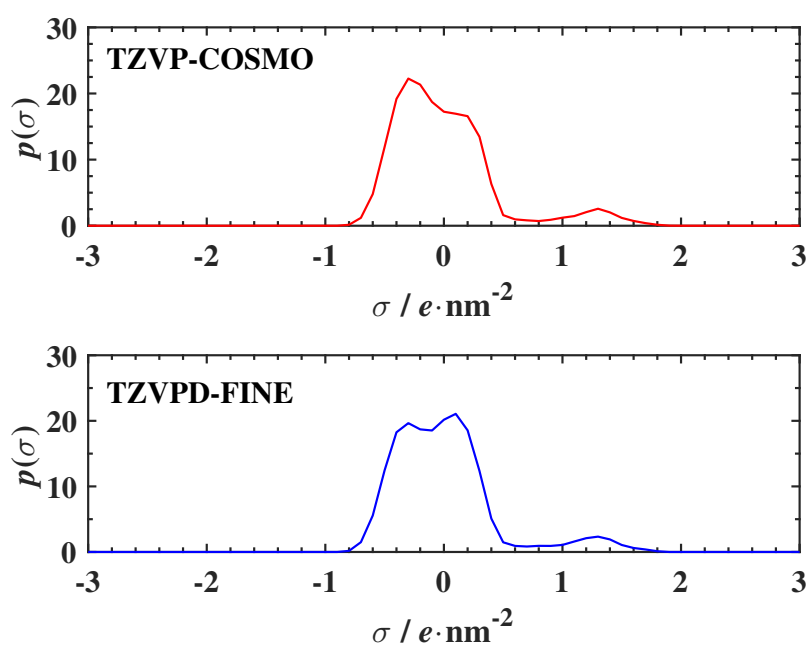
**Figure S298.**  $\sigma$ -profiles of L-(-)-menthol (CAS-RN: 2216-51-5) obtained from screening charge distributions calculated at the BP-TZVP-COSMO level and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



**Figure S299.**  $\sigma$ -profiles of linalool (CAS-RN: 78-70-6) obtained from screening charge distributions calculated at the BP-TZVP-COSMO level and BP-TZVPD-FINE levels. Thick lines are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



**Figure S300.**  $\sigma$ -profiles of thymol (CAS-RN: 89-83-8) obtained from screening charge distributions calculated at the BP-TZVP-COSMO level and BP-TZVPD-FINE levels. Thick lines are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).



**Figure S301.**  $\sigma$ -profiles of  $\alpha$ -pinene oxide (CAS-RN: 1686-14-2) obtained from screening charge distributions calculated at the BP-TZVP-COSMO level and BP-TZVPD-FINE levels. Thick line are designated by the lowest-energy conformer, whereas lighter lines correspond to the remaining conformations (if available).