Rational computing of energy levels for organic electronics: the case of 2-benzylidene-1,3-indandiones

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Supplementary material 1A. Full Reference 44 from the main article

M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski and D. J. Fox, Gaussian, Inc., 2009.

Supplementary material 1B. Notes on Gaussian 09 keywords usage.

Upon reviewer's advice, we place here some more detailed explanation of calculation input parameters and keywords we used to obtain the results of current study. Solvent (ACN) was modeled with *SCRF=CPCM* keyword, using all default parameters (UFF atomic radii system with scaling factor 1.1, etc.). Non-equilibrium solvation was forced by specifying parameter *SCRF=Read* in both ΔSCF jobs and putting in additional input section *NonEq=Write* for neutral state calculation and *NonEq=Read* for the ionic one.

Supplementary material 1C. Details of factor analysis

Calculations were performed in the form of full factorial experiment what allows to assess standard deviation of data by evaluating hidden replicates. The last appear due to multiple occurrence of certain factor levels (e.g., no *CPCM* is level 0 and using *CPCM* is level 1) in experiments with different values for other parameters. Well-known statistical methods allows for no even extracting these standard error, but also pointing out most influential factors. This is done by transforming the matrix of experimental or calculated values to the matrix of effects. In our case, these initial values are slopes, intercepts, R^2's and times for correlations between experimental data and value computed by method corresponding to a certain element in the matrix mentioned, i.e., to a combination of factors at certain levels. This combination is termed a treatment. For example, if we have factors d (diffuse functions – three levels), p (polarization functions on H atoms – two levels) and z (double or triple zeta – also two levels), we will have treatments 3×2×2 = 12 treatments 0, d_1, d_2, p_1, p_1d_1, p_1d_2, z_1, z_1d_1, z_1d_2, z_1p_1, $z_1p_1d_1$ and $z_1p_1d_2$. When there is z in the name of a treatment, extra valence function is used, etc.

The values after the transformation are effects of corresponding factors. Linear effects are calculated simply as level differences; continuing with our example, effect from adding extra valence functions to computation model is defined as

$$6Z = z_1 + z_1d_1 + z_1d_2 + z_1p_1 + z_1p_1d_1 + z_1p_1d_2 - 0 - d_1 - d_2 - p_1 - p_1d_1 - p_1d_2. \quad \text{(S1)}$$

Factor six appears because the effect Z itself is average of all differences. The effects can be plotted as a function of level number, normalized to the number of levels. In this example, at $x = 0$ the effect has value 0, but at $x = 1$ it has value Z. For factors where there are more than two levels, there is also quadratic effect, which can be defined as the difference with prediction of linear effect at $x = ½$ and the actual experimental (or calculated) value of corresponding treatment. For d then, the quadratic effect D^q is

$$8D^q = z_1 - 2z_1d_1 + z_1d_2 + z_1p_1 - 2z_1p_1d_1 + z_1p_1d_2 + 0 - 2d_1 + d_2 + p_1 - 2p_1d_1 + p_1d_2. \qquad \text{(S2)}$$

Factor 2 appears because number of positive terms must equal that of negative ones (as D^q still needs to be like a certain weighted average in its meaning). The factor of 8 consists of 4 for four combinations of other parameters and of 2 for bringing it in accordance with the definition above. Example of one single difference is then $\frac{z_1 + z_1d_2}{2} - z_1d_1$, where the first term is the average value of two end levels of effect, what corresponds to $x = ½$ for absolutely linear factor. Analogically, cubic effect for a factor with four levels can be defined as a difference between the value predicted by quadratic factor equation and the actual value at $x = ⅔$. Calculation of effects can be straightforwardly expressed as matrix operation involving transposition, so it is easily done by modern software (such as R).

After all the effects are calculated, one could also determine which ones are significant. Daniel's test[1] allows for this by plotting effects along with normal distribution quantiles (as on Q–Q plot). Then, effect points that are distributed along the diagonal with small departure from it are interpreted as corresponding to insignificant factors, because these effect are indistinguishable from random ones (of which normal distribution is descriptive). An example of Daniel's test plot is available on Figure S1.

There is, of course, some degree of subjectivity in determining which effect is far from the diagonal and which is not. We tried to develop an automated criterion for this that is not to be refitted for different cases (for example, when dealing with I or with A). The fact that we performed full factorial experiment helped us in that we had plenty of data points (namely 216). We defined a central region in the plot, spreading from –1 to 1 on the axis of normal distribution quantiles, which we considered to contain only insignificant data points, and calculated maximum separation of data points in this region along effects quantiles axis. All effect points distance of which from the point next to them and closer to the central region is more than N times this separation were treated significant, N being determined empirically to avoid obvious inconsistencies for all cases studied. For our case, this was $N = 5$.

From the rest of effects, treatments can be calculated back by inverse matrix operations. These are the 'corrected data' we present in Results section. Further information on factor analysis is available in reference [2].

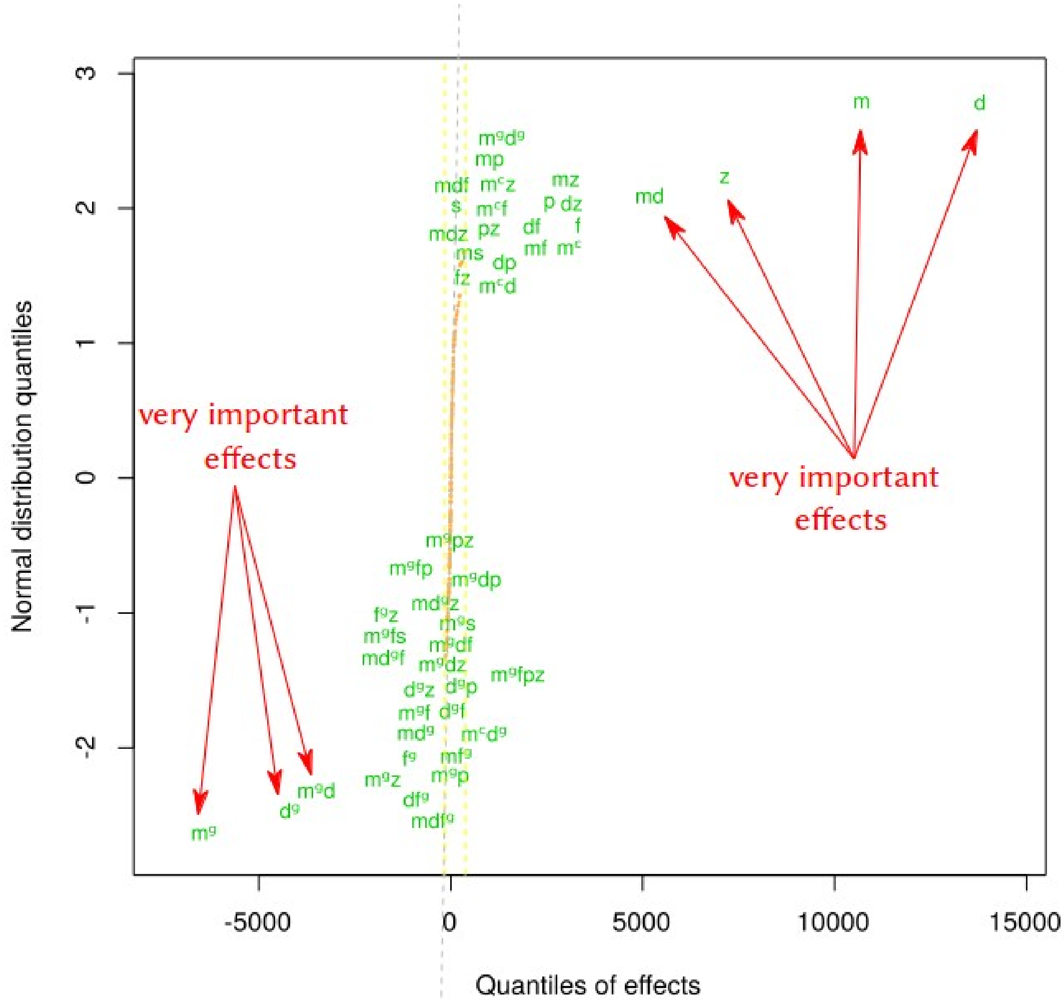


Figure S1. Example of Daniel's test plot for ionization energy calculations (computation time). Points of effects that are treated insignificant are shown in orange; others are shown by caption which may be shifted for better readability. Yellow lines are boundaries of the region points in which were treated as corresponding to insignificant factors (probably random noise or molecule-specific effects).

Now, let us look on example in our actual study. We have four-level factor *m* (for methodology) with levels that correspond to orbital energy approach ($x = 0$), vertical ΔSCF ($x = ⅓$), adiabatic ΔSCF ($x = ⅔$) and adiabatic ΔSCF with ZPVC applied ($x = 1$). Computation times of the first two levels should differ severely (at least twice), while the difference between $x = ⅓$ and $x = ⅔$ should be much smaller and that between $x = ⅔$ and $x = 1$ is nought because ZPVC is obtained from geometry optimization, time of which is not included in this analysis. Logically, the whole picture is well-represented by the quadratic effect, and the cubic one is treated to be insignificant in further analysis (see Figure S2). Therefore, in the 'corrected data' points of adiabatic ΔSCF and of adiabatic ΔSCF with ZPVC applied will not be strictly equal, as the corresponding small effect was removed during the analysis. Some other similar perturbations were noticed during the analysis of results.

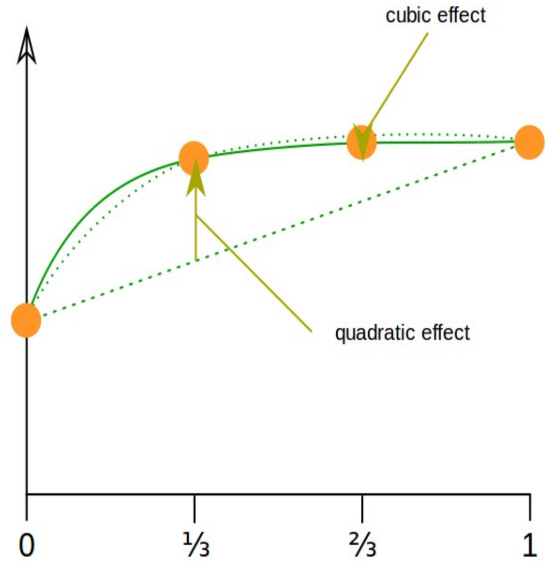


Figure S2. Comparative size of quadratic and cubic effects of *m* factor in the present study.

We can eventually note that the full analysis for single dataset (*I* or *A*) took approximately 45 seconds on *Intel Core i3*, single thread.

References

(S1) Daniel, C. *Technometrics* **1959**, *1* (4), 311.

(S2) Mead, R.; Gilmour, S. G.; Mead, A. *Statistical Principles for the Design of Experiments: Applications to Real Experiments*; 2012.

Supplementary material 1D. Results of factor analysis including the factor of solvent.

(see next two pages)

The reason to exclude the factor of solvent from the tables presented in the main article was to facilitate better comprehension of results. As the impact of solvent factor is by much the greatest, it can unreasonably distract reader's attention from the remaining factors, what was in fact observed in the initial communication with reviewers. The data were subsequently recalculated without the factor of solvent, with no obvious change in results observed. This assures us of robustness of the chosen factorial analysis methodology which compensates the possible bias in main factor by recognizing significant interactions (see Supplementary material 1C).

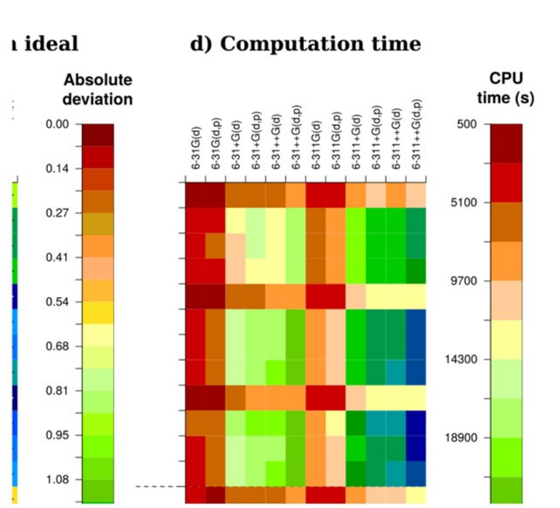


Figure S3. Results of factor-effect analysis for ionization energy (see also Figure 3 in the main article). Sign of deviation is indicated in each cell of the tables. Cell coloring represents the quality of results, with reddish brown corresponding to high precision mountains and dark blue – to deep discord seas

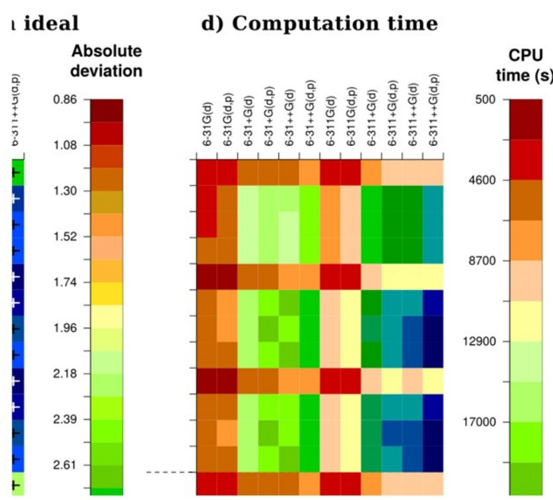


Figure S4. Results of factor-effect analysis for electron affinity (see also Figure 6 in the main article). Sign of deviation is indicated in each cell of the tables. Cell coloring represents the quality of results, with reddish brown corresponding to high precision mountains and dark blue – to deep discord seas

Supplementary material 2A. Numerical values of figures of merit

The data presented here are plotted on Figures 3 and 6 in the main material without giving the values themselves. The data consists of deviations of regression parameters from their ideal description (1 for slope and $R^2$and 0 for intercept), as well as of computation time (or CPU time, as this is time renormalized as on single CPU core, which is output by default in *Gaussian 09* on *GNU/Linux*. Also included is the mean absolute deviation (MAD) of computed results from the experimental CV data, which was not considered during the analysis but is probably interesting to the research community. We would like to note, in addition, that there is good (almost linear) correlation between the MAD and the intercept for data points studied.
Results of computations themselves are available from the authors upon e-mail request.

Part 1. Double-zeta basis sets

Table S1. Figures of merit for ionization energy for double-zeta basis sets

(a) Slope (experimental ~ calculated)

	6-31G(d)	6-31G(d,p)	6-31+G(d)	6-31+G(d,p)	6-31++G(d)	6-31++G(d,p)
CAM-B3LYP // CAM-B3LYP/6-31G(d,p), adiabatic ΔSCF & ZPVC & CPCM	-0.03867221	-0.04057056	-0.05125301	-0.05315136	-0.05166967	-0.05356801
CAM-B3LYP // CAM-B3LYP/6-31G(d,p), adiabatic ΔSCF & CPCM	-0.06815481	-0.06960693	-0.08007179	-0.08152391	-0.07855321	-0.08000533
CAM-B3LYP // CAM-B3LYP/6-31G(d,p), vertical ΔSCF & CPCM	-0.17075558	-0.17176148	-0.18492768	-0.18593358	-0.18439279	-0.18539869
CAM-B3LYP // CAM-B3LYP/6-31G(d,p), orbital energies & CPCM	-0.09642779	-0.09698748	-0.11335441	-0.1139141	-0.11430263	-0.11486231
CAM-B3LYP // B3LYP/6-31G(d,p), adiabatic ΔSCF & ZPVC & CPCM	-0.03491013	-0.03680847	-0.04717572	-0.04907406	-0.04727716	-0.04917551
CAM-B3LYP // B3LYP/6-31G(d,p), adiabatic ΔSCF & CPCM	-0.06860328	-0.0700554	-0.08020505	-0.08165717	-0.07837126	-0.07982338
CAM-B3LYP // B3LYP/6-31G(d,p), vertical ΔSCF & CPCM	-0.1545747	-0.1555806	-0.16843158	-0.16943749	-0.16758149	-0.16858739
CAM-B3LYP // B3LYP/6-31G(d,p), orbital energies & CPCM	-0.07688002	-0.07743971	-0.09349144	-0.09405112	-0.09412444	-0.09468412
B3LYP // B3LYP/6-31G(d,p), adiabatic ΔSCF & ZPVC & CPCM	0.03456385	0.03266551	0.02261347	0.02071513	0.02282724	0.02092889
B3LYP // B3LYP/6-31G(d,p), adiabatic ΔSCF & CPCM	-0.00363498	-0.0050871	-0.01492154	-0.01637367	-0.01277254	-0.01422466
B3LYP // B3LYP/6-31G(d,p), vertical ΔSCF & CPCM	-0.09984134	-0.10084724	-0.11338302	-0.11438892	-0.11221771	-0.11322361
B3LYP // B3LYP/6-31G(d,p), orbital energies & CPCM	0.01570568	0.01514599	-0.00059053	-0.00115021	-0.00090832	-0.001468
CAM-B3LYP // CAM-B3LYP/6-31G(d,p), adiabatic ΔSCF & ZPVC	-0.21318692	-0.21508526	-0.20963799	-0.21153634	-0.20908047	-0.21097881
CAM-B3LYP // CAM-B3LYP/6-31G(d,p), adiabatic ΔSCF	-0.23118107	-0.23263319	-0.22958015	-0.23103228	-0.22969922	-0.23115134
CAM-B3LYP // CAM-B3LYP/6-31G(d,p), vertical ΔSCF	-0.23653388	-0.23753979	-0.23718809	-0.23819399	-0.23829084	-0.23929675
CAM-B3LYP // CAM-B3LYP/6-31G(d,p), orbital energies	-0.15021649	-0.15077618	-0.15101339	-0.15157307	-0.15098742	-0.1515471
CAM-B3LYP // B3LYP/6-31G(d,p), adiabatic ΔSCF & ZPVC	-0.20936701	-0.21126535	-0.20550287	-0.20740122	-0.20463014	-0.20652848
CAM-B3LYP // B3LYP/6-31G(d,p), adiabatic ΔSCF	-0.23309487	-0.234547	-0.23117875	-0.23263087	-0.2309826	-0.23243473
CAM-B3LYP // B3LYP/6-31G(d,p), vertical ΔSCF	-0.22334149	-0.2243474	-0.22368049	-0.22468639	-0.22446804	-0.22547394
CAM-B3LYP // B3LYP/6-31G(d,p), orbital energies	-0.13518038	-0.13574007	-0.13566207	-0.13622175	-0.13532089	-0.13588057
B3LYP // B3LYP/6-31G(d,p), adiabatic ΔSCF & ZPVC	-0.16269294	-0.16459128	-0.15851359	-0.16041193	-0.15732564	-0.15922399
B3LYP // B3LYP/6-31G(d,p), adiabatic ΔSCF	-0.18940332	-0.19085544	-0.18717199	-0.18862411	-0.18666063	-0.18811276
B3LYP // B3LYP/6-31G(d,p), vertical ΔSCF	-0.18836172	-0.18936762	-0.1883855	-0.18939141	-0.18885784	-0.18986375
B3LYP // B3LYP/6-31G(d,p), orbital energies	-0.0608251	-0.06138479	-0.06099158	-0.06155126	-0.06033519	-0.06089487

(b) Intercept (experimental ~ calculated)

	6-31G(d)	6-31G(d,p)	6-31+G(d)	6-31+G(d,p)	6-31++G(d)	6-31++G(d,p)
CAM-B3LYP // CAM-B3LYP/6-31G(d,p), adiabatic ΔSCF & ZPVC & CPCM	0.19040809	0.20987086	0.25986583	0.2793286	0.25482483	0.2742876
CAM-B3LYP // CAM-B3LYP/6-31G(d,p), adiabatic ΔSCF & CPCM	0.36212136	0.37750615	0.4347557	0.45014049	0.43721225	0.45259704
CAM-B3LYP // CAM-B3LYP/6-31G(d,p), vertical ΔSCF & CPCM	1.09433974	1.10564655	1.1737412	1.18504802	1.17047835	1.18178516
CAM-B3LYP // CAM-B3LYP/6-31G(d,p), orbital energies & CPCM	1.6142127	1.62144153	1.72329787	1.7305267	1.72042468	1.72765352
CAM-B3LYP // B3LYP/6-31G(d,p), adiabatic ΔSCF & ZPVC & CPCM	0.13166995	0.15113272	0.19913102	0.21859379	0.19209334	0.21155612
CAM-B3LYP // B3LYP/6-31G(d,p), adiabatic ΔSCF & CPCM	0.33196204	0.34734683	0.40259971	0.4179845	0.40305959	0.41844439
CAM-B3LYP // B3LYP/6-31G(d,p), vertical ΔSCF & CPCM	0.96708918	0.97839599	1.04449398	1.05580079	1.03923446	1.05054127
CAM-B3LYP // B3LYP/6-31G(d,p), orbital energies & CPCM	1.50344764	1.51067647	1.61053613	1.61776497	1.60566628	1.61289511
B3LYP // B3LYP/6-31G(d,p), adiabatic ΔSCF & ZPVC & CPCM	-0.2763005	-0.25683772	-0.21083609	-0.19137332	-0.21987044	-0.20040766
B3LYP // B3LYP/6-31G(d,p), adiabatic ΔSCF & CPCM	-0.05804507	-0.04266028	0.01059594	0.02598073	0.00905915	0.02444394
B3LYP // B3LYP/6-31G(d,p), vertical ΔSCF & CPCM	0.71558064	0.72688745	0.79098877	0.80229558	0.78373257	0.79503938
B3LYP // B3LYP/6-31G(d,p), orbital energies & CPCM	0.46813852	0.47536735	0.57323034	0.58045918	0.56636382	0.57359265
CAM-B3LYP // CAM-B3LYP/6-31G(d,p), adiabatic ΔSCF & ZPVC	1.57822078	1.59768355	1.50168847	1.52115124	1.4987113	1.51817407
CAM-B3LYP // CAM-B3LYP/6-31G(d,p), adiabatic ΔSCF	1.66360235	1.67898714	1.61297468	1.62835947	1.60660812	1.62199292
CAM-B3LYP // CAM-B3LYP/6-31G(d,p), vertical ΔSCF	1.68070827	1.69201509	1.65239472	1.66370153	1.65585574	1.66716255
CAM-B3LYP // CAM-B3LYP/6-31G(d,p), orbital energies	1.9714613	1.97869013	1.94254529	1.94977412	1.94972481	1.95695364
CAM-B3LYP // B3LYP/6-31G(d,p), adiabatic ΔSCF & ZPVC	1.55428961	1.57375239	1.47576064	1.49522341	1.4707868	1.49024957
CAM-B3LYP // B3LYP/6-31G(d,p), adiabatic ΔSCF	1.67646274	1.69184753	1.62383841	1.6392232	1.61547518	1.63085997
CAM-B3LYP // B3LYP/6-31G(d,p), vertical ΔSCF	1.57847086	1.58977768	1.54816064	1.55946745	1.54962499	1.5609318
CAM-B3LYP // B3LYP/6-31G(d,p), orbital energies	1.88081246	1.88804129	1.84989978	1.85712861	1.85508263	1.86231146
B3LYP // B3LYP/6-31G(d,p), adiabatic ΔSCF & ZPVC	1.29327908	1.31274185	1.21275343	1.23221621	1.20578293	1.2252457
B3LYP // B3LYP/6-31G(d,p), adiabatic ΔSCF	1.44162827	1.45701306	1.38700726	1.40239205	1.37664737	1.39203216
B3LYP // B3LYP/6-31G(d,p), vertical ΔSCF	1.46412838	1.47543519	1.43182149	1.4431283	1.43128917	1.44259598
B3LYP // B3LYP/6-31G(d,p), orbital energies	0.97777248	0.98500131	0.94486313	0.95209196	0.94804931	0.95527814

(c) R^2(experimental ~ calculated)

	6-31G(d)	6-31G(d,p)	6-31+G(d)	6-31+G(d,p)	6-31++G(d)	6-31++G(d,p)
CAM-B3LYP // CAM-B3LYP/6-31G(d,p), adiabatic ΔSCF & ZPVC & CPCM	-0.01151136	-0.01079299	-0.01042549	-0.00970712	-0.00957107	-0.00885269
CAM-B3LYP // CAM-B3LYP/6-31G(d,p), adiabatic ΔSCF & CPCM	-0.01222669	-0.01188195	-0.00949792	-0.00915318	-0.0094601	-0.00911536
CAM-B3LYP // CAM-B3LYP/6-31G(d,p), vertical ΔSCF & CPCM	-0.01681548	-0.01684437	-0.01885024	-0.01887914	-0.01848958	-0.01851848
CAM-B3LYP // CAM-B3LYP/6-31G(d,p), orbital energies & CPCM	-0.01376125	-0.01416378	-0.01467156	-0.01507409	-0.01454624	-0.01494877
CAM-B3LYP // B3LYP/6-31G(d,p), adiabatic ΔSCF & ZPVC & CPCM	-0.01191763	-0.01119926	-0.01051833	-0.00979996	-0.01010872	-0.00939034

CAM-B3LYP // B3LYP/6-31G(d,p), adiabatic ΔSCF & CPCM	-0.01209346	-0.01174872	-0.00943475	-0.00909001	-0.00971973	-0.00937499
CAM-B3LYP // B3LYP/6-31G(d,p), vertical ΔSCF & CPCM	-0.01652045	-0.01654935	-0.01900876	-0.01903765	-0.01884889	-0.01887779
CAM-B3LYP // B3LYP/6-31G(d,p), orbital energies & CPCM	-0.01317288	-0.01357541	-0.01492022	-0.01532275	-0.01487368	-0.01527621
B3LYP // B3LYP/6-31G(d,p), adiabatic ΔSCF & ZPVC & CPCM	-0.02072848	-0.0200101	-0.0204735	-0.01975512	-0.02044997	-0.01973159
B3LYP // B3LYP/6-31G(d,p), adiabatic ΔSCF & CPCM	-0.02078075	-0.02043601	-0.01867801	-0.01833327	-0.01926622	-0.01892148
B3LYP // B3LYP/6-31G(d,p), vertical ΔSCF & CPCM	-0.03040328	-0.03043217	-0.03285921	-0.0328881	-0.03291972	-0.03294861
B3LYP // B3LYP/6-31G(d,p), orbital energies & CPCM	-0.01425962	-0.01466215	-0.01538624	-0.01578877	-0.01547723	-0.01587976
CAM-B3LYP // CAM-B3LYP/6-31G(d,p), adiabatic ΔSCF & ZPVC	-0.09137392	-0.0917783	-0.07390131	-0.07430569	-0.07358708	-0.07399146
CAM-B3LYP // CAM-B3LYP/6-31G(d,p), adiabatic ΔSCF	-0.08939798	-0.08942873	-0.07271126	-0.07274201	-0.07203149	-0.07206223
CAM-B3LYP // CAM-B3LYP/6-31G(d,p), vertical ΔSCF	-0.06384772	-0.06350483	-0.05184154	-0.05149865	-0.05193766	-0.05159477
CAM-B3LYP // CAM-B3LYP/6-31G(d,p), orbital energies	-0.06779626	-0.06707974	-0.04872764	-0.04801112	-0.04909548	-0.04837895
CAM-B3LYP // B3LYP/6-31G(d,p), adiabatic ΔSCF & ZPVC	-0.09324389	-0.09364827	-0.07545785	-0.07586223	-0.07558843	-0.07599281
CAM-B3LYP // B3LYP/6-31G(d,p), adiabatic ΔSCF	-0.09037924	-0.09040999	-0.07376257	-0.07379332	-0.0734056	-0.07343635
CAM-B3LYP // B3LYP/6-31G(d,p), vertical ΔSCF	-0.06190628	-0.06156339	-0.05035364	-0.05001075	-0.05065056	-0.05030767
CAM-B3LYP // B3LYP/6-31G(d,p), orbital energies	-0.06502553	-0.064309	-0.04679394	-0.04607742	-0.04724057	-0.04652404
B3LYP // B3LYP/6-31G(d,p), adiabatic ΔSCF & ZPVC	-0.09614456	-0.09654894	-0.07950283	-0.07990722	-0.08001949	-0.08042388
B3LYP // B3LYP/6-31G(d,p), adiabatic ΔSCF	-0.09337356	-0.09340431	-0.07731287	-0.07734361	-0.07725912	-0.07728987
B3LYP // B3LYP/6-31G(d,p), vertical ΔSCF	-0.07408385	-0.07374096	-0.06249884	-0.06215595	-0.06301613	-0.06267324
B3LYP // B3LYP/6-31G(d,p), orbital energies	-0.0675286	-0.06681208	-0.04867629	-0.04795977	-0.04926043	-0.04854391

(d) Computation time as on single CPU core

	6-31G(d)	6-31G(d,p)	6-31+G(d)	6-31+G(d,p)	6-31++G(d)	6-31++G(d,p)
CAM-B3LYP // CAM-B3LYP/6-31G(d,p), adiabatic ΔSCF & ZPVC & CPCM	5866.995	7065.252	16967.385	19443.191	20057.084	22624.92
CAM-B3LYP // CAM-B3LYP/6-31G(d,p), adiabatic ΔSCF & CPCM	6270.954	7490.674	17265.165	20405.555	20106.605	23982.147
CAM-B3LYP // CAM-B3LYP/6-31G(d,p), vertical ΔSCF & CPCM	6802.612	7462.488	18347.964	20928.511	21220.101	24535.798
CAM-B3LYP // CAM-B3LYP/6-31G(d,p), orbital energies & CPCM	2566.679	2085.403	6510.954	7307.226	7623.506	8511.808
CAM-B3LYP // B3LYP/6-31G(d,p), adiabatic ΔSCF & ZPVC & CPCM	6154.834	7460.951	16770.091	19353.757	20874.899	23550.594
CAM-B3LYP // B3LYP/6-31G(d,p), adiabatic ΔSCF & CPCM	6544.406	7656.267	16515.073	19547.605	19536.191	23303.874
CAM-B3LYP // B3LYP/6-31G(d,p), vertical ΔSCF & CPCM	6131.165	6683.181	16791.433	19264.12	19684.686	22892.524
CAM-B3LYP // B3LYP/6-31G(d,p), orbital energies & CPCM	2667.058	2293.641	6541.577	7445.709	8193.555	9189.716
B3LYP // B3LYP/6-31G(d,p), adiabatic ΔSCF & ZPVC & CPCM	4954.821	6368.797	12719.856	15411.381	15474.683	18258.237
B3LYP // B3LYP/6-31G(d,p), adiabatic ΔSCF & CPCM	5859.138	6863.14	12939.187	15863.859	14272.907	17932.731
B3LYP // B3LYP/6-31G(d,p), vertical ΔSCF & CPCM	5030.13	5474.287	13436.252	15801.08	14981.561	18081.54
B3LYP // B3LYP/6-31G(d,p), orbital energies & CPCM	2866.982	2601.425	5800.699	6812.69	7121.055	8225.075
CAM-B3LYP // CAM-B3LYP/6-31G(d,p), adiabatic ΔSCF & ZPVC	4947.972	6146.229	16048.362	18524.168	19138.061	21705.897
CAM-B3LYP // CAM-B3LYP/6-31G(d,p), adiabatic ΔSCF	4528.889	5748.609	15523.099	18663.49	18364.54	22240.082
CAM-B3LYP // CAM-B3LYP/6-31G(d,p), vertical ΔSCF	5408.439	6068.314	16953.791	19534.337	19825.927	23141.625

CAM-B3LYP // CAM-B3LYP/6-31G(d,p), orbital energies	2691.331	2210.055	6635.606	7431.879	7748.159	8636.461
CAM-B3LYP // B3LYP/6-31G(d,p), adiabatic ΔSCF & ZPVC	4989.72	6295.837	15604.978	18188.643	19709.786	22385.48
CAM-B3LYP // B3LYP/6-31G(d,p), adiabatic ΔSCF	5048.431	6160.292	15019.098	18051.63	18040.217	21807.9
CAM-B3LYP // B3LYP/6-31G(d,p), vertical ΔSCF	4983.082	5535.098	15643.35	18116.037	18536.603	21744.441
CAM-B3LYP // B3LYP/6-31G(d,p), orbital energies	2545.62	2172.203	6420.139	7324.271	8072.117	9068.278
B3LYP // B3LYP/6-31G(d,p), adiabatic ΔSCF & ZPVC	3543.617	4957.593	11308.652	14000.177	14063.479	16847.033
B3LYP // B3LYP/6-31G(d,p), adiabatic ΔSCF	4609.254	5613.255	11689.302	14613.975	13023.023	16682.846
B3LYP // B3LYP/6-31G(d,p), vertical ΔSCF	4128.137	4572.294	12534.259	14899.087	14079.568	17179.547
B3LYP // B3LYP/6-31G(d,p), orbital energies	2499.454	2233.896	5433.17	6445.161	6753.526	7857.546

(e) Mean absolute deviations of results

	6-31G(d)	6-31G(d,p)	6-31+G(d)	6-31+G(d,p)	6-31++G(d)	6-31++G(d,p)
CAM-B3LYP // CAM-B3LYP/6-31G(d,p), adiabatic ΔSCF & ZPVC & CPCM	0.08016845	0.0589036	0.09093756	0.06967271	0.09176451	0.07049967
CAM-B3LYP // CAM-B3LYP/6-31G(d,p), adiabatic ΔSCF & CPCM	0.08370303	0.07173428	0.1000014	0.08803266	0.10570978	0.09374103
CAM-B3LYP // CAM-B3LYP/6-31G(d,p), vertical ΔSCF & CPCM	0.09125821	0.08858556	0.10792262	0.10524997	0.11334919	0.11067653
CAM-B3LYP // CAM-B3LYP/6-31G(d,p), orbital energies & CPCM	1.10358193	1.11020537	1.11544914	1.12207258	1.11543066	1.1220541
CAM-B3LYP // B3LYP/6-31G(d,p), adiabatic ΔSCF & ZPVC & CPCM	0.11762804	0.09636319	0.1280518	0.10678696	0.12853342	0.10726857
CAM-B3LYP // B3LYP/6-31G(d,p), adiabatic ΔSCF & CPCM	0.12242841	0.11045966	0.13321821	0.12124946	0.13341801	0.12144926
CAM-B3LYP // B3LYP/6-31G(d,p), vertical ΔSCF & CPCM	0.09717604	0.09450338	0.10833187	0.10565922	0.10824986	0.10557721
CAM-B3LYP // B3LYP/6-31G(d,p), orbital energies & CPCM	1.09437894	1.10100239	1.10590082	1.11252426	1.10553699	1.11216043
B3LYP // B3LYP/6-31G(d,p), adiabatic ΔSCF & ZPVC & CPCM	0.08503632	0.06377147	0.09511474	0.0738499	0.09525101	0.07398617
B3LYP // B3LYP/6-31G(d,p), adiabatic ΔSCF & CPCM	0.09472323	0.08275448	0.10000445	0.0880357	0.09469568	0.08272693
B3LYP // B3LYP/6-31G(d,p), vertical ΔSCF & CPCM	0.08499792	0.08232527	0.09064518	0.08797253	0.0850546	0.08238195
B3LYP // B3LYP/6-31G(d,p), orbital energies & CPCM	0.54828823	0.55491167	0.55946476	0.5660882	0.55875559	0.56537903
CAM-B3LYP // CAM-B3LYP/6-31G(d,p), adiabatic ΔSCF & ZPVC	0.27844102	0.28626999	0.21160275	0.21943172	0.21193322	0.21976219
CAM-B3LYP // CAM-B3LYP/6-31G(d,p), adiabatic ΔSCF	0.25239444	0.25988456	0.20480318	0.2122933	0.21025124	0.21774136
CAM-B3LYP // CAM-B3LYP/6-31G(d,p), vertical ΔSCF	0.22784535	0.23499663	0.19433787	0.20148915	0.19974029	0.20689157
CAM-B3LYP // CAM-B3LYP/6-31G(d,p), orbital energies	1.16574767	1.17256011	1.14116074	1.14797318	1.1413543	1.14816673
CAM-B3LYP // B3LYP/6-31G(d,p), adiabatic ΔSCF & ZPVC	0.27759907	0.28542804	0.21041546	0.21824443	0.21040058	0.21822955
CAM-B3LYP // B3LYP/6-31G(d,p), adiabatic ΔSCF	0.25945582	0.26694594	0.20635598	0.21384611	0.20629547	0.21378559
CAM-B3LYP // B3LYP/6-31G(d,p), vertical ΔSCF	0.21176769	0.21891897	0.17275164	0.17990292	0.17264548	0.17979676
CAM-B3LYP // B3LYP/6-31G(d,p), orbital energies	1.15476581	1.16157824	1.12983354	1.13664597	1.12968174	1.13649418
B3LYP // B3LYP/6-31G(d,p), adiabatic ΔSCF & ZPVC	0.29331388	0.30114284	0.22578492	0.23361389	0.2254247	0.23325367
B3LYP // B3LYP/6-31G(d,p), adiabatic ΔSCF	0.27256489	0.28005502	0.21395649	0.22144661	0.2083874	0.21587752
B3LYP // B3LYP/6-31G(d,p), vertical ΔSCF	0.30729814	0.31444942	0.26277352	0.2699248	0.25715879	0.26431007
B3LYP // B3LYP/6-31G(d,p), orbital energies	0.62045896	0.6272714	0.59518134	0.60199378	0.59468421	0.60149664

Table S2. Figures of merit for electron affinity for double-zeta basis sets

(a) Slope (experimental ~ calculated)

	6-31G(d)	6-31G(d,p)	6-31+G(d)	6-31+G(d,p)	6-31++G(d)	6-31++G(d,p)
CAM-B3LYP // CAM-B3LYP/6-31G(d,p), adiabatic ΔSCF & ZPVC & CPCM	-0.2354337	-0.2357822	-0.236747	-0.2370955	-0.2372198	-0.2375683
CAM-B3LYP // CAM-B3LYP/6-31G(d,p), adiabatic ΔSCF & CPCM	-0.2651746	-0.2633541	-0.2663337	-0.2645133	-0.2650797	-0.2632593
CAM-B3LYP // CAM-B3LYP/6-31G(d,p), vertical ΔSCF & CPCM	-0.202348	-0.1993226	-0.193685	-0.1906596	-0.1934242	-0.1903989
CAM-B3LYP // CAM-B3LYP/6-31G(d,p), orbital energies & CPCM	-0.2972298	-0.2939636	-0.2962741	-0.293008	-0.2969134	-0.2936472
CAM-B3LYP // B3LYP/6-31G(d,p), adiabatic ΔSCF & ZPVC & CPCM	-0.2329718	-0.2333204	-0.2377838	-0.2381323	-0.2378365	-0.238185
CAM-B3LYP // B3LYP/6-31G(d,p), adiabatic ΔSCF & CPCM	-0.267857	-0.2660366	-0.2732998	-0.2714793	-0.2724105	-0.2705901
CAM-B3LYP // B3LYP/6-31G(d,p), vertical ΔSCF & CPCM	-0.2262022	-0.2231769	-0.2218228	-0.2187975	-0.2219269	-0.2189015
CAM-B3LYP // B3LYP/6-31G(d,p), orbital energies & CPCM	-0.3194439	-0.3161777	-0.3219869	-0.3187207	-0.3222061	-0.3189399
B3LYP // B3LYP/6-31G(d,p), adiabatic ΔSCF & ZPVC & CPCM	-0.3333371	-0.3336856	-0.3416477	-0.3419962	-0.3412803	-0.3416289
B3LYP // B3LYP/6-31G(d,p), adiabatic ΔSCF & CPCM	-0.3593958	-0.3575753	-0.3691221	-0.3673016	-0.3685977	-0.3667773
B3LYP // B3LYP/6-31G(d,p), vertical ΔSCF & CPCM	-0.3217256	-0.3187003	-0.3216298	-0.3186044	-0.3220986	-0.3190733
B3LYP // B3LYP/6-31G(d,p), orbital energies & CPCM	-0.3673905	-0.3641244	-0.3734322	-0.370166	-0.3732313	-0.3699652
CAM-B3LYP // CAM-B3LYP/6-31G(d,p), adiabatic ΔSCF & ZPVC	-0.4067767	-0.4053714	-0.4114473	-0.4100421	-0.4110398	-0.4096345
CAM-B3LYP // CAM-B3LYP/6-31G(d,p), adiabatic ΔSCF	-0.4332812	-0.4308762	-0.4359369	-0.4335319	-0.4357579	-0.4333528
CAM-B3LYP // CAM-B3LYP/6-31G(d,p), vertical ΔSCF	-0.5583282	-0.5558875	-0.5453856	-0.5429448	-0.5442398	-0.541799
CAM-B3LYP // CAM-B3LYP/6-31G(d,p), orbital energies	-0.5807703	-0.5792579	-0.5717164	-0.570204	-0.5714684	-0.569956
CAM-B3LYP // B3LYP/6-31G(d,p), adiabatic ΔSCF & ZPVC	-0.4083554	-0.4069501	-0.4138901	-0.4124849	-0.4130268	-0.4116215
CAM-B3LYP // B3LYP/6-31G(d,p), adiabatic ΔSCF	-0.435174	-0.4327689	-0.4394786	-0.4370736	-0.4396287	-0.4372237
CAM-B3LYP // B3LYP/6-31G(d,p), vertical ΔSCF	-0.5644153	-0.5619746	-0.5531216	-0.5506809	-0.552305	-0.5498642
CAM-B3LYP // B3LYP/6-31G(d,p), orbital energies	-0.5881013	-0.586589	-0.5799116	-0.5783992	-0.5792078	-0.5776954
B3LYP // B3LYP/6-31G(d,p), adiabatic ΔSCF & ZPVC	-0.4673905	-0.4659853	-0.4737893	-0.4723841	-0.4724702	-0.471065
B3LYP // B3LYP/6-31G(d,p), adiabatic ΔSCF	-0.4887048	-0.4862997	-0.4946584	-0.4922534	-0.4951377	-0.4927326
B3LYP // B3LYP/6-31G(d,p), vertical ΔSCF	-0.5854334	-0.5829926	-0.5757886	-0.5733479	-0.5753011	-0.5728604
B3LYP // B3LYP/6-31G(d,p), orbital energies	-0.6027876	-0.6012752	-0.5954619	-0.5939495	-0.5943023	-0.5927899

(b) Intercept (experimental ~ calculated)

	6-31G(d)	6-31G(d,p)	6-31+G(d)	6-31+G(d,p)	6-31++G(d)	6-31++G(d,p)
CAM-B3LYP // CAM-B3LYP/6-31G(d,p), adiabatic ΔSCF & ZPVC & CPCM	1.072604	1.072604	0.9413951	0.9413951	0.9321969	0.9321969
CAM-B3LYP // CAM-B3LYP/6-31G(d,p), adiabatic ΔSCF & CPCM	1.228968	1.228968	1.1129554	1.1129554	1.1079969	1.1079969
CAM-B3LYP // CAM-B3LYP/6-31G(d,p), vertical ΔSCF & CPCM	2.74129	2.74129	2.5845278	2.5845278	2.5826682	2.5826682
CAM-B3LYP // CAM-B3LYP/6-31G(d,p), orbital energies & CPCM	4.139847	4.139847	4.0786012	4.0786012	4.0817296	4.0817296

CAM-B3LYP // B3LYP/6-31G(d,p), adiabatic ΔSCF & ZPVC & CPCM	1.022085	1.022085	0.923111	0.923111	0.9210392	0.9210392
CAM-B3LYP // B3LYP/6-31G(d,p), adiabatic ΔSCF & CPCM	1.2038	1.2038	1.1152358	1.1152358	1.1126177	1.1126177
CAM-B3LYP // B3LYP/6-31G(d,p), vertical ΔSCF & CPCM	2.687433	2.687433	2.553332	2.553332	2.5490265	2.5490265
CAM-B3LYP // B3LYP/6-31G(d,p), orbital energies & CPCM	4.070372	4.070372	4.027002	4.027002	4.0228982	4.0228982
B3LYP // B3LYP/6-31G(d,p), adiabatic ΔSCF & ZPVC & CPCM	1.364785	1.364785	1.2875641	1.2875641	1.2821381	1.2821381
B3LYP // B3LYP/6-31G(d,p), adiabatic ΔSCF & CPCM	1.506981	1.506981	1.4423705	1.4423705	1.4385992	1.4385992
B3LYP // B3LYP/6-31G(d,p), vertical ΔSCF & CPCM	2.79741	2.79741	2.6894649	2.6894649	2.686207	2.686207
B3LYP // B3LYP/6-31G(d,p), orbital energies & CPCM	2.22034	2.22034	2.2053264	2.2053264	2.2044713	2.2044713
CAM-B3LYP // CAM-B3LYP/6-31G(d,p), adiabatic ΔSCF & ZPVC	3.705053	3.705053	3.5621646	3.5621646	3.5650692	3.5650692
CAM-B3LYP // CAM-B3LYP/6-31G(d,p), adiabatic ΔSCF	3.76486	3.76486	3.6331101	3.6331101	3.6348161	3.6348161
CAM-B3LYP // CAM-B3LYP/6-31G(d,p), vertical ΔSCF	3.99433	3.99433	3.8941406	3.8941406	3.8950175	3.8950175
CAM-B3LYP // CAM-B3LYP/6-31G(d,p), orbital energies	4.070174	4.070174	4.0226652	4.0226652	4.0225665	4.0225665
CAM-B3LYP // B3LYP/6-31G(d,p), adiabatic ΔSCF & ZPVC	3.707479	3.707479	3.5656968	3.5656968	3.5652121	3.5652121
CAM-B3LYP // B3LYP/6-31G(d,p), adiabatic ΔSCF	3.764801	3.764801	3.6363585	3.6363585	3.6368762	3.6368762
CAM-B3LYP // B3LYP/6-31G(d,p), vertical ΔSCF	3.942234	3.942234	3.8475534	3.8475534	3.849443	3.849443
CAM-B3LYP // B3LYP/6-31G(d,p), orbital energies	4.029002	4.029002	3.9892034	3.9892034	3.9923184	3.9923184
B3LYP // B3LYP/6-31G(d,p), adiabatic ΔSCF & ZPVC	3.6558	3.6558	3.5256054	3.5256054	3.5322123	3.5322123
B3LYP // B3LYP/6-31G(d,p), adiabatic ΔSCF	3.713286	3.713286	3.5916457	3.5916457	3.5944687	3.5944687
B3LYP // B3LYP/6-31G(d,p), vertical ΔSCF	3.912516	3.912516	3.81985	3.81985	3.8192587	3.8192587
B3LYP // B3LYP/6-31G(d,p), orbital energies	2.871125	2.871125	2.8285554	2.8285554	2.8244032	2.8244032

(c) R^2(experimental ~ calculated)

	6-31G(d)	6-31G(d,p)	6-31+G(d)	6-31+G(d,p)	6-31++G(d)	6-31++G(d,p)
CAM-B3LYP // CAM-B3LYP/6-31G(d,p), adiabatic ΔSCF & ZPVC & CPCM	-0.1585181	-0.1575951	-0.1373759	-0.1364529	-0.1368871	-0.1359641
CAM-B3LYP // CAM-B3LYP/6-31G(d,p), adiabatic ΔSCF & CPCM	-0.1594013	-0.1590937	-0.1394523	-0.1391446	-0.1367862	-0.1364786
CAM-B3LYP // CAM-B3LYP/6-31G(d,p), vertical ΔSCF & CPCM	-0.1653536	-0.1656612	-0.1399301	-0.1402377	-0.1388455	-0.1391531
CAM-B3LYP // CAM-B3LYP/6-31G(d,p), orbital energies & CPCM	-0.1496033	-0.1505263	-0.1366296	-0.1375526	-0.136493	-0.1374159
CAM-B3LYP // B3LYP/6-31G(d,p), adiabatic ΔSCF & ZPVC & CPCM	-0.1625283	-0.1616053	-0.1410153	-0.1400923	-0.1378097	-0.1368867
CAM-B3LYP // B3LYP/6-31G(d,p), adiabatic ΔSCF & CPCM	-0.1603399	-0.1600323	-0.1417869	-0.1414793	-0.138171	-0.1378634
CAM-B3LYP // B3LYP/6-31G(d,p), vertical ΔSCF & CPCM	-0.1602405	-0.1605481	-0.1370508	-0.1373585	-0.1358542	-0.1361618
CAM-B3LYP // B3LYP/6-31G(d,p), orbital energies & CPCM	-0.1445871	-0.14551	-0.133756	-0.134679	-0.133416	-0.134339
B3LYP // B3LYP/6-31G(d,p), adiabatic ΔSCF & ZPVC & CPCM	-0.1493738	-0.1484508	-0.1329581	-0.1320351	-0.1325039	-0.1315809
B3LYP // B3LYP/6-31G(d,p), adiabatic ΔSCF & CPCM	-0.1468998	-0.1465922	-0.1335354	-0.1332277	-0.1327621	-0.1324544
B3LYP // B3LYP/6-31G(d,p), vertical ΔSCF & CPCM	-0.1536448	-0.1539525	-0.1348059	-0.1351135	-0.135614	-0.1359217
B3LYP // B3LYP/6-31G(d,p), orbital energies & CPCM	-0.1317403	-0.1326632	-0.123493	-0.124416	-0.123391	-0.1243139
CAM-B3LYP // CAM-B3LYP/6-31G(d,p), adiabatic ΔSCF & ZPVC	-0.1728352	-0.1719122	-0.1580014	-0.1570784	-0.1607772	-0.1598542

CAM-B3LYP // CAM-B3LYP/6-31G(d,p), adiabatic ΔSCF	-0.1757559	-0.1754483	-0.158909	-0.1586014	-0.1615123	-0.1612046
CAM-B3LYP // CAM-B3LYP/6-31G(d,p), vertical ΔSCF	-0.3144477	-0.3147554	-0.2833241	-0.2836318	-0.2839175	-0.2842252
CAM-B3LYP // CAM-B3LYP/6-31G(d,p), orbital energies	-0.2868632	-0.2877862	-0.2621852	-0.2631082	-0.2629333	-0.2638562
CAM-B3LYP // B3LYP/6-31G(d,p), adiabatic ΔSCF & ZPVC	-0.1802687	-0.1793458	-0.1640087	-0.1630857	-0.1630124	-0.1620894
CAM-B3LYP // B3LYP/6-31G(d,p), adiabatic ΔSCF	-0.18112	-0.1808123	-0.1646138	-0.1643061	-0.1652118	-0.1649041
CAM-B3LYP // B3LYP/6-31G(d,p), vertical ΔSCF	-0.306104	-0.3064117	-0.2761589	-0.2764666	-0.2755849	-0.2758926
CAM-B3LYP // B3LYP/6-31G(d,p), orbital energies	-0.2783784	-0.2793014	-0.2547877	-0.2557107	-0.2542771	-0.2552
B3LYP // B3LYP/6-31G(d,p), adiabatic ΔSCF & ZPVC	-0.1882647	-0.1873417	-0.1760466	-0.1751236	-0.1767463	-0.1758233
B3LYP // B3LYP/6-31G(d,p), adiabatic ΔSCF	-0.1876119	-0.1873042	-0.1752388	-0.1749312	-0.1776241	-0.1773165
B3LYP // B3LYP/6-31G(d,p), vertical ΔSCF	-0.2893432	-0.2896509	-0.2626935	-0.2630012	-0.263069	-0.2633766
B3LYP // B3LYP/6-31G(d,p), orbital energies	-0.2711758	-0.2720988	-0.2491136	-0.2500365	-0.2477855	-0.2487084

(d) Computation time as on single CPU core

	6-31G(d)	6-31G(d,p)	6-31+G(d)	6-31+G(d,p)	6-31++G(d)	6-31++G(d,p)
CAM-B3LYP // CAM-B3LYP/6-31G(d,p), adiabatic ΔSCF & ZPVC & CPCM	5116.596	5922.852	16407.079	18449.101	19129.174	22406.963
CAM-B3LYP // CAM-B3LYP/6-31G(d,p), adiabatic ΔSCF & CPCM	5177.584	6690.497	16922.572	19443.345	18454.196	21982.829
CAM-B3LYP // CAM-B3LYP/6-31G(d,p), vertical ΔSCF & CPCM	5332.721	6521.572	16113.649	18082.453	18732.893	21481.65
CAM-B3LYP // CAM-B3LYP/6-31G(d,p), orbital energies & CPCM	2348.21	2182.278	5952.602	6338.716	7143.646	8081.807
CAM-B3LYP // B3LYP/6-31G(d,p), adiabatic ΔSCF & ZPVC & CPCM	5749.945	6556.201	16275.27	18317.292	19109.93	22387.719
CAM-B3LYP // B3LYP/6-31G(d,p), adiabatic ΔSCF & CPCM	5611.343	7124.256	16814.453	19335.226	18681.921	22210.554
CAM-B3LYP // B3LYP/6-31G(d,p), vertical ΔSCF & CPCM	5533.815	6722.666	15996.145	17964.949	19174.514	21923.271
CAM-B3LYP // B3LYP/6-31G(d,p), orbital energies & CPCM	2283.564	2117.632	5792.638	6178.752	7766.087	8704.248
B3LYP // B3LYP/6-31G(d,p), adiabatic ΔSCF & ZPVC & CPCM	5108.062	5914.318	13308.901	15350.923	14696.797	17974.586
B3LYP // B3LYP/6-31G(d,p), adiabatic ΔSCF & CPCM	4079.171	5592.084	13181.075	15701.849	13825.059	17353.693
B3LYP // B3LYP/6-31G(d,p), vertical ΔSCF & CPCM	4513.699	5702.549	13098.103	15066.907	15276.267	18025.025
B3LYP // B3LYP/6-31G(d,p), orbital energies & CPCM	3177.848	3011.916	5032.276	5418.391	6228.801	7166.962
CAM-B3LYP // CAM-B3LYP/6-31G(d,p), adiabatic ΔSCF & ZPVC	5116.596	5922.852	16407.079	18449.101	19129.174	22406.963
CAM-B3LYP // CAM-B3LYP/6-31G(d,p), adiabatic ΔSCF	5177.584	6690.497	16922.572	19443.345	18454.196	21982.829
CAM-B3LYP // CAM-B3LYP/6-31G(d,p), vertical ΔSCF	5332.721	6521.572	16113.649	18082.453	18732.893	21481.65
CAM-B3LYP // CAM-B3LYP/6-31G(d,p), orbital energies	2348.21	2182.278	5952.602	6338.716	7143.646	8081.807
CAM-B3LYP // B3LYP/6-31G(d,p), adiabatic ΔSCF & ZPVC	5749.945	6556.201	16275.27	18317.292	19109.93	22387.719
CAM-B3LYP // B3LYP/6-31G(d,p), adiabatic ΔSCF	5611.343	7124.256	16814.453	19335.226	18681.921	22210.554
CAM-B3LYP // B3LYP/6-31G(d,p), vertical ΔSCF	5533.815	6722.666	15996.145	17964.949	19174.514	21923.271
CAM-B3LYP // B3LYP/6-31G(d,p), orbital energies	2283.564	2117.632	5792.638	6178.752	7766.087	8704.248
B3LYP // B3LYP/6-31G(d,p), adiabatic ΔSCF & ZPVC	5108.062	5914.318	13308.901	15350.923	14696.797	17974.586
B3LYP // B3LYP/6-31G(d,p), adiabatic ΔSCF	4079.171	5592.084	13181.075	15701.849	13825.059	17353.693
B3LYP // B3LYP/6-31G(d,p), vertical ΔSCF	4513.699	5702.549	13098.103	15066.907	15276.267	18025.025

B3LYP // B3LYP/6-31G(d,p), orbital energies	3177.848	3011.916	5032.276	5418.391	6228.801	7166.962

(e) Mean absolute deviations of results

	6-31G(d)	6-31G(d,p)	6-31+G(d)	6-31+G(d,p)	6-31++G(d)	6-31++G(d,p)
CAM-B3LYP // CAM-B3LYP/6-31G(d,p), adiabatic ΔSCF & ZPVC & CPCM	0.1944329	0.1949625	0.05156102	0.05209058	0.0489931	0.04952266
CAM-B3LYP // CAM-B3LYP/6-31G(d,p), adiabatic ΔSCF & CPCM	0.2928564	0.293386	0.11981151	0.12034107	0.1233385	0.12386805
CAM-B3LYP // CAM-B3LYP/6-31G(d,p), vertical ΔSCF & CPCM	2.4576815	2.4582111	2.27141453	2.27194408	2.27478717	2.27531673
CAM-B3LYP // CAM-B3LYP/6-31G(d,p), orbital energies & CPCM	4.2361333	4.2366629	4.16515381	4.16568337	4.16278545	4.163315
CAM-B3LYP // B3LYP/6-31G(d,p), adiabatic ΔSCF & ZPVC & CPCM	0.1567382	0.1572677	0.06395998	0.06448954	0.06242539	0.06295495
CAM-B3LYP // B3LYP/6-31G(d,p), adiabatic ΔSCF & CPCM	0.2460973	0.2466269	0.09670568	0.09723524	0.08979076	0.09032032
CAM-B3LYP // B3LYP/6-31G(d,p), vertical ΔSCF & CPCM	2.3518215	2.352351	2.17419049	2.17472005	2.16706928	2.16759884
CAM-B3LYP // B3LYP/6-31G(d,p), orbital energies & CPCM	4.1564658	4.1569953	4.09052839	4.09105795	4.0890375	4.08956706
B3LYP // B3LYP/6-31G(d,p), adiabatic ΔSCF & ZPVC & CPCM	0.1282497	0.1287793	0.09535841	0.09588797	0.10465035	0.10517991
B3LYP // B3LYP/6-31G(d,p), adiabatic ΔSCF & CPCM	0.2032013	0.2037309	0.08725609	0.08778565	0.07969248	0.08022204
B3LYP // B3LYP/6-31G(d,p), vertical ΔSCF & CPCM	2.2869363	2.2874659	2.12773456	2.12826412	2.1199127	2.12044226
B3LYP // B3LYP/6-31G(d,p), orbital energies & CPCM	1.2728098	1.2733394	1.22170775	1.2222373	1.23088752	1.23141708
CAM-B3LYP // CAM-B3LYP/6-31G(d,p), adiabatic ΔSCF & ZPVC	3.5870136	3.5875432	3.34775242	3.34828197	3.34881385	3.34934341
CAM-B3LYP // CAM-B3LYP/6-31G(d,p), adiabatic ΔSCF	3.6729727	3.6735023	3.4441516	3.44468116	3.4429166	3.44344615
CAM-B3LYP // CAM-B3LYP/6-31G(d,p), vertical ΔSCF	4.1393618	4.1398913	3.91913249	3.91966204	3.91809441	3.91862397
CAM-B3LYP // CAM-B3LYP/6-31G(d,p), orbital energies	4.3255542	4.3260838	4.22362723	4.22415679	4.22594204	4.2264716
CAM-B3LYP // B3LYP/6-31G(d,p), adiabatic ΔSCF & ZPVC	3.5910392	3.5915688	3.34885206	3.34938162	3.34627017	3.34679973
CAM-B3LYP // B3LYP/6-31G(d,p), adiabatic ΔSCF	3.6802504	3.6807799	3.44949917	3.45002873	3.44201631	3.44254587
CAM-B3LYP // B3LYP/6-31G(d,p), vertical ΔSCF	4.0324554	4.0329849	3.81393322	3.81446277	3.80668408	3.80721364
CAM-B3LYP // B3LYP/6-31G(d,p), orbital energies	4.2437261	4.2442556	4.14978476	4.15031431	4.14856663	4.14909618
B3LYP // B3LYP/6-31G(d,p), adiabatic ΔSCF & ZPVC	3.4525178	3.4530474	3.21719794	3.2177275	3.22076593	3.22129549
B3LYP // B3LYP/6-31G(d,p), adiabatic ΔSCF	3.5458012	3.5463308	3.32291317	3.32344273	3.31897565	3.31950521
B3LYP // B3LYP/6-31G(d,p), vertical ΔSCF	3.9522233	3.9527528	3.74520145	3.74573101	3.74153445	3.74206401
B3LYP // B3LYP/6-31G(d,p), orbital energies	1.3572876	1.3578171	1.28112512	1.28165468	1.28616725	1.28669681

Part 2. Triple-zeta basis sets

Table S3. Figures of merit for ionization energy for triple-zeta basis sets

(a) Slope (experimental ~ calculated)

	6-311G(d)	6-311G(d,p)	6-311+G(d)	6-311+G(d,p)	6-311++G(d)	6-311++G(d,p)
CAM-B3LYP // CAM-B3LYP/6-31G(d,p), adiabatic ΔSCF & ZPVC & CPCM	-0.044790252	-0.046688595	-0.049526591	-0.051424934	-0.051242336	-0.053140679
CAM-B3LYP // CAM-B3LYP/6-31G(d,p), adiabatic ΔSCF & CPCM	-0.072921098	-0.074373221	-0.076516867	-0.07796899	-0.075820622	-0.077272745
CAM-B3LYP // CAM-B3LYP/6-31G(d,p), vertical ΔSCF & CPCM	-0.175591446	-0.176597349	-0.180965579	-0.181971482	-0.180776276	-0.181782179

CAM-B3LYP // CAM-B3LYP/6-31G(d,p), orbital energies & CPCM	-0.102754556	-0.103314239	-0.110406458	-0.110966141	-0.111223502	-0.111783186
CAM-B3LYP // B3LYP/6-31G(d,p), adiabatic ΔSCF & ZPVC & CPCM	-0.041028168	-0.042926511	-0.045449297	-0.047347639	-0.046849832	-0.048748175
CAM-B3LYP // B3LYP/6-31G(d,p), adiabatic ΔSCF & CPCM	-0.073369567	-0.07482169	-0.076650127	-0.07810225	-0.075638672	-0.077090795
CAM-B3LYP // B3LYP/6-31G(d,p), vertical ΔSCF & CPCM	-0.15941056	-0.160416464	-0.164469484	-0.165475387	-0.163964971	-0.164970874
CAM-B3LYP // B3LYP/6-31G(d,p), orbital energies & CPCM	-0.083206786	-0.083766469	-0.090543479	-0.091103162	-0.091045313	-0.091604997
B3LYP // B3LYP/6-31G(d,p), adiabatic ΔSCF & ZPVC & CPCM	0.028445812	0.026547469	0.024339893	0.02244155	0.023254567	0.021356224
B3LYP // B3LYP/6-31G(d,p), adiabatic ΔSCF & CPCM	-0.00840127	-0.009853393	-0.01136662	-0.012818743	-0.010039956	-0.011492079
B3LYP // B3LYP/6-31G(d,p), vertical ΔSCF & CPCM	-0.104677201	-0.105683105	-0.109420915	-0.110426818	-0.108601193	-0.109607096
B3LYP // B3LYP/6-31G(d,p), orbital energies & CPCM	0.009378914	0.008819231	0.002357431	0.001797748	0.002170806	0.001611122
CAM-B3LYP // CAM-B3LYP/6-31G(d,p), adiabatic ΔSCF & ZPVC	-0.216789811	-0.218688154	-0.20931837	-0.211216713	-0.209761483	-0.211659826
CAM-B3LYP // CAM-B3LYP/6-31G(d,p), adiabatic ΔSCF	-0.23343221	-0.234884334	-0.22743203	-0.228884153	-0.228074982	-0.229527105
CAM-B3LYP // CAM-B3LYP/6-31G(d,p), vertical ΔSCF	-0.238854601	-0.239860504	-0.234632783	-0.235638687	-0.235782678	-0.236788581
CAM-B3LYP // CAM-B3LYP/6-31G(d,p), orbital energies	-0.154028107	-0.154587791	-0.14947223	-0.150031913	-0.149016643	-0.149576326
CAM-B3LYP // B3LYP/6-31G(d,p), adiabatic ΔSCF & ZPVC	-0.212969901	-0.214868244	-0.205183251	-0.207081594	-0.205311154	-0.207209497
CAM-B3LYP // B3LYP/6-31G(d,p), adiabatic ΔSCF	-0.235346016	-0.236798139	-0.229030625	-0.230482748	-0.229358368	-0.230810491
CAM-B3LYP // B3LYP/6-31G(d,p), vertical ΔSCF	-0.225662212	-0.226668115	-0.221125185	-0.222131088	-0.22195987	-0.222965773
CAM-B3LYP // B3LYP/6-31G(d,p), orbital energies	-0.138991996	-0.139551679	-0.134120909	-0.134680592	-0.133350112	-0.133909795
B3LYP // B3LYP/6-31G(d,p), adiabatic ΔSCF & ZPVC	-0.166295827	-0.16819417	-0.158193967	-0.16009231	-0.158006661	-0.159905004
B3LYP // B3LYP/6-31G(d,p), adiabatic ΔSCF	-0.191654463	-0.193106587	-0.185023863	-0.186475986	-0.185036396	-0.186488519
B3LYP // B3LYP/6-31G(d,p), vertical ΔSCF	-0.190682437	-0.19168834	-0.1858302	-0.186836103	-0.186349675	-0.187355578
B3LYP // B3LYP/6-31G(d,p), orbital energies	-0.064636718	-0.065196402	-0.059450422	-0.060010105	-0.058364415	-0.058924099

(b) Intercept (experimental ~ calculated)

	6-311G(d)	6-311G(d,p)	6-311+G(d)	6-311+G(d,p)	6-311++G(d)	6-311++G(d,p)
CAM-B3LYP // CAM-B3LYP/6-31G(d,p), adiabatic ΔSCF & ZPVC & CPCM	0.20979028	0.241987123	0.20561497	0.2378118	0.21282941	0.24502625
CAM-B3LYP // CAM-B3LYP/6-31G(d,p), adiabatic ΔSCF & CPCM	0.38207283	0.410191691	0.3763756	0.4044945	0.38638906	0.41450793
CAM-B3LYP // CAM-B3LYP/6-31G(d,p), vertical ΔSCF & CPCM	1.1267641	1.150804977	1.12313546	1.1471763	1.122731	1.14677188
CAM-B3LYP // CAM-B3LYP/6-31G(d,p), orbital energies & CPCM	1.67101356	1.690976457	1.69237009	1.712333	1.68765678	1.70761968
CAM-B3LYP // B3LYP/6-31G(d,p), adiabatic ΔSCF & ZPVC & CPCM	0.15105214	0.183248977	0.14488016	0.177077	0.15009793	0.18229477
CAM-B3LYP // B3LYP/6-31G(d,p), adiabatic ΔSCF & CPCM	0.35191351	0.380032373	0.34421961	0.3723385	0.35223641	0.38035527
CAM-B3LYP // B3LYP/6-31G(d,p), vertical ΔSCF & CPCM	0.99951354	1.023554423	0.99388824	1.0179291	0.9914871	1.01552799
CAM-B3LYP // B3LYP/6-31G(d,p), orbital energies & CPCM	1.56024849	1.580211393	1.57960836	1.5995713	1.57289837	1.59286127
B3LYP // B3LYP/6-31G(d,p), adiabatic ΔSCF & ZPVC & CPCM	-0.25691831	-0.224721464	-0.26508695	-0.2328901	-0.26186585	-0.22966901
B3LYP // B3LYP/6-31G(d,p), adiabatic ΔSCF & CPCM	-0.03809359	-0.009974733	-0.04778416	-0.0196653	-0.04176404	-0.01364517
B3LYP // B3LYP/6-31G(d,p), vertical ΔSCF & CPCM	0.748005	0.772045878	0.74038303	0.7644239	0.73598522	0.7600261
B3LYP // B3LYP/6-31G(d,p), orbital energies & CPCM	0.52493937	0.544902271	0.54230257	0.5622655	0.53359591	0.55355881

CAM-B3LYP // CAM-B3LYP/6-31G(d,p), adiabatic ΔSCF & ZPVC	1.57244514	1.604641982	1.4610169	1.4932137	1.46829442	1.50049126
CAM-B3LYP // CAM-B3LYP/6-31G(d,p), adiabatic ΔSCF	1.65839599	1.686514855	1.56817387	1.5962927	1.56736347	1.59548233
CAM-B3LYP // CAM-B3LYP/6-31G(d,p), vertical ΔSCF	1.68797481	1.71201569	1.61536827	1.6394092	1.61968693	1.64372781
CAM-B3LYP // CAM-B3LYP/6-31G(d,p), orbital energies	2.00310433	2.023067227	1.92519681	1.9451597	1.92853543	1.94849834
CAM-B3LYP // B3LYP/6-31G(d,p), adiabatic ΔSCF & ZPVC	1.54851398	1.580710819	1.43508907	1.4672859	1.44036992	1.47256676
CAM-B3LYP // B3LYP/6-31G(d,p), adiabatic ΔSCF	1.67125639	1.69937525	1.5790376	1.6071565	1.57623053	1.60434939
CAM-B3LYP // B3LYP/6-31G(d,p), vertical ΔSCF	1.5857374	1.609778278	1.51113419	1.5351751	1.51345618	1.53749706
CAM-B3LYP // B3LYP/6-31G(d,p), orbital energies	1.91245548	1.932418385	1.8325513	1.8525142	1.83389325	1.85385615
B3LYP // B3LYP/6-31G(d,p), adiabatic ΔSCF & ZPVC	1.28750344	1.319700282	1.17208187	1.2042787	1.17536604	1.20756288
B3LYP // B3LYP/6-31G(d,p), adiabatic ΔSCF	1.43642191	1.464540776	1.34220645	1.3703253	1.33740272	1.36552158
B3LYP // B3LYP/6-31G(d,p), vertical ΔSCF	1.47139491	1.495435795	1.39479504	1.4188359	1.39512036	1.41916124
B3LYP // B3LYP/6-31G(d,p), orbital energies	1.0094155	1.029378404	0.92751465	0.9474775	0.92685993	0.94682284

(c) R^2(experimental ~ calculated)

	6-311G(d)	6-311G(d,p)	6-311+G(d)	6-311+G(d,p)	6-311++G(d)	6-311++G(d,p)
CAM-B3LYP // CAM-B3LYP/6-31G(d,p), adiabatic ΔSCF & ZPVC & CPCM	-0.009709893	-0.009241711	-0.010144339	-0.009676158	-0.009376496	-0.008908315
CAM-B3LYP // CAM-B3LYP/6-31G(d,p), adiabatic ΔSCF & CPCM	-0.010223614	-0.010129069	-0.009015162	-0.008920617	-0.009063919	-0.008969374
CAM-B3LYP // CAM-B3LYP/6-31G(d,p), vertical ΔSCF & CPCM	-0.014610804	-0.014889895	-0.018165884	-0.018444976	-0.017891799	-0.018170891
CAM-B3LYP // CAM-B3LYP/6-31G(d,p), orbital energies & CPCM	-0.011354974	-0.012007701	-0.013785602	-0.01443833	-0.013746855	-0.014399583
CAM-B3LYP // B3LYP/6-31G(d,p), adiabatic ΔSCF & ZPVC & CPCM	-0.00981376	-0.009345578	-0.009934776	-0.009466594	-0.00961174	-0.009143559
CAM-B3LYP // B3LYP/6-31G(d,p), adiabatic ΔSCF & CPCM	-0.009989585	-0.00989504	-0.008851189	-0.008756644	-0.009222749	-0.009128204
CAM-B3LYP // B3LYP/6-31G(d,p), vertical ΔSCF & CPCM	-0.014416578	-0.01469567	-0.018425201	-0.018704293	-0.018351913	-0.018631004
CAM-B3LYP // B3LYP/6-31G(d,p), orbital energies & CPCM	-0.011069002	-0.01172173	-0.014336659	-0.014989387	-0.014376702	-0.01502943
B3LYP // B3LYP/6-31G(d,p), adiabatic ΔSCF & ZPVC & CPCM	-0.018322205	-0.017854023	-0.01958754	-0.019119359	-0.019650586	-0.019182405
B3LYP // B3LYP/6-31G(d,p), adiabatic ΔSCF & CPCM	-0.018576072	-0.018481527	-0.01799365	-0.017899105	-0.018668435	-0.01857389
B3LYP // B3LYP/6-31G(d,p), vertical ΔSCF & CPCM	-0.028400203	-0.028679294	-0.032376452	-0.032655543	-0.032523535	-0.032802627
B3LYP // B3LYP/6-31G(d,p), orbital energies & CPCM	-0.012458151	-0.013110879	-0.015105088	-0.015757815	-0.015282648	-0.015935376
CAM-B3LYP // CAM-B3LYP/6-31G(d,p), adiabatic ΔSCF & ZPVC	-0.087263163	-0.086510457	-0.07593642	-0.075183714	-0.075496455	-0.074743749
CAM-B3LYP // CAM-B3LYP/6-31G(d,p), adiabatic ΔSCF	-0.085085622	-0.083959279	-0.074544766	-0.073418424	-0.073739259	-0.072612916
CAM-B3LYP // CAM-B3LYP/6-31G(d,p), vertical ΔSCF	-0.059333754	-0.057833775	-0.053473444	-0.051973465	-0.053443827	-0.051943848
CAM-B3LYP // CAM-B3LYP/6-31G(d,p), orbital energies	-0.063080695	-0.06120708	-0.050157946	-0.04828433	-0.050400044	-0.048526429
CAM-B3LYP // B3LYP/6-31G(d,p), adiabatic ΔSCF & ZPVC	-0.088830729	-0.088078023	-0.077190555	-0.076437849	-0.077195399	-0.076442693
CAM-B3LYP // B3LYP/6-31G(d,p), adiabatic ΔSCF	-0.085966076	-0.084839734	-0.075495277	-0.074368934	-0.075012572	-0.073886229
CAM-B3LYP // B3LYP/6-31G(d,p), vertical ΔSCF	-0.057493117	-0.055993138	-0.052086349	-0.05058637	-0.052257529	-0.05075755
CAM-B3LYP // B3LYP/6-31G(d,p), orbital energies	-0.060612369	-0.058738753	-0.048526648	-0.046653032	-0.048847537	-0.046973921
B3LYP // B3LYP/6-31G(d,p), adiabatic ΔSCF & ZPVC	-0.09142899	-0.090676284	-0.080933136	-0.08018043	-0.081324061	-0.080571354

B3LYP // B3LYP/6-31G(d,p), adiabatic ΔSCF	-0.088859598	-0.087733255	-0.078944771	-0.077818429	-0.078765293	-0.07763895
B3LYP // B3LYP/6-31G(d,p), vertical ΔSCF	-0.06977149	-0.068271511	-0.064332348	-0.062832369	-0.0647239	-0.063223921
B3LYP // B3LYP/6-31G(d,p), orbital energies	-0.063417845	-0.06154423	-0.050711403	-0.048837788	-0.05116981	-0.049296194

(d) Computation time as on single CPU core

	6-311G(d)	6-311G(d,p)	6-311+G(d)	6-311+G(d,p)	6-311++G(d)	6-311++G(d,p)
CAM-B3LYP // CAM-B3LYP/6-31G(d,p), adiabatic ΔSCF & ZPVC & CPCM	10321.059	11810.313	27303.841	30070.65	31249.148	34107.98
CAM-B3LYP // CAM-B3LYP/6-31G(d,p), adiabatic ΔSCF & CPCM	9180.632	12566.557	26371.284	31677.88	31260.58	37302.33
CAM-B3LYP // CAM-B3LYP/6-31G(d,p), vertical ΔSCF & CPCM	10680.388	13506.468	27236.326	31983.08	31848.66	37330.56
CAM-B3LYP // CAM-B3LYP/6-31G(d,p), orbital energies & CPCM	4560.01	4369.731	10829.108	11916.38	11874.297	13053.6
CAM-B3LYP // B3LYP/6-31G(d,p), adiabatic ΔSCF & ZPVC & CPCM	10381.293	12373.137	26878.943	30148.34	31839.358	35200.78
CAM-B3LYP // B3LYP/6-31G(d,p), adiabatic ΔSCF & CPCM	9621.21	12504.544	25788.319	30592.32	30857.292	36396.45
CAM-B3LYP // B3LYP/6-31G(d,p), vertical ΔSCF & CPCM	10176.067	12499.557	25846.92	30091.08	30480.371	35459.68
CAM-B3LYP // B3LYP/6-31G(d,p), orbital energies & CPCM	4432.785	4745.096	10632.127	12221.99	12216.741	13898.63
B3LYP // B3LYP/6-31G(d,p), adiabatic ΔSCF & ZPVC & CPCM	7923.19	10417.625	21570.618	25342.6	25181.052	29045.06
B3LYP // B3LYP/6-31G(d,p), adiabatic ΔSCF & CPCM	8072.583	10453.328	21349.073	25650.49	24730.649	29767.22
B3LYP // B3LYP/6-31G(d,p), vertical ΔSCF & CPCM	8211.673	10032.573	21628.38	25369.95	24913.887	29390.61
B3LYP // B3LYP/6-31G(d,p), orbital energies & CPCM	3374.619	4189.52	8633.159	10725.61	9886.151	12070.63
CAM-B3LYP // CAM-B3LYP/6-31G(d,p), adiabatic ΔSCF & ZPVC	9402.035	10891.29	26384.818	29151.62	30330.125	33188.96
CAM-B3LYP // CAM-B3LYP/6-31G(d,p), adiabatic ΔSCF	7438.567	10824.491	24629.219	29935.81	29518.515	35560.26
CAM-B3LYP // CAM-B3LYP/6-31G(d,p), vertical ΔSCF	9286.215	12112.295	25842.152	30588.9	30454.487	35936.39
CAM-B3LYP // CAM-B3LYP/6-31G(d,p), orbital energies	4684.662	4494.384	10953.76	12041.03	11998.949	13178.25
CAM-B3LYP // B3LYP/6-31G(d,p), adiabatic ΔSCF & ZPVC	9216.179	11208.024	25713.829	28983.22	30674.244	34035.67
CAM-B3LYP // B3LYP/6-31G(d,p), adiabatic ΔSCF	8125.235	11008.57	24292.344	29096.35	29361.317	34900.47
CAM-B3LYP // B3LYP/6-31G(d,p), vertical ΔSCF	9027.984	11351.473	24698.837	28943	29332.288	34311.6
CAM-B3LYP // B3LYP/6-31G(d,p), orbital energies	4311.346	4623.657	10510.689	12100.55	12095.302	13777.19
B3LYP // B3LYP/6-31G(d,p), adiabatic ΔSCF & ZPVC	6511.986	9006.421	20159.414	23931.4	23769.848	27633.86
B3LYP // B3LYP/6-31G(d,p), adiabatic ΔSCF	6822.699	9203.444	20099.189	24400.6	23480.765	28517.33
B3LYP // B3LYP/6-31G(d,p), vertical ΔSCF	7309.68	9130.581	20726.388	24467.96	24011.894	28488.62
B3LYP // B3LYP/6-31G(d,p), orbital energies	3007.091	3821.992	8265.63	10358.08	9518.622	11703.1

(e) Mean absolute deviations of results

	6-311G(d)	6-311G(d,p)	6-311+G(d)	6-311+G(d,p)	6-311++G(d)	6-311++G(d,p)
CAM-B3LYP // CAM-B3LYP/6-31G(d,p), adiabatic ΔSCF & ZPVC & CPCM	0.076916	0.05565116	0.10935983	0.08809499	0.10969561	0.08843077
CAM-B3LYP // CAM-B3LYP/6-31G(d,p), adiabatic ΔSCF & CPCM	0.08832354	0.07635479	0.11184682	0.09987807	0.11739147	0.10542272

CAM-B3LYP // CAM-B3LYP/6-31G(d,p), vertical ΔSCF & CPCM	0.10375167	0.10107902	0.11319117	0.11051852	0.11878146	0.11610881
CAM-B3LYP // CAM-B3LYP/6-31G(d,p), orbital energies & CPCM	1.12394834	1.13057178	1.11414083	1.12076427	1.11461353	1.12123697
CAM-B3LYP // B3LYP/6-31G(d,p), adiabatic ΔSCF & ZPVC & CPCM	0.11437559	0.09311075	0.14647408	0.12520924	0.14646452	0.12519967
CAM-B3LYP // B3LYP/6-31G(d,p), adiabatic ΔSCF & CPCM	0.12704891	0.11508016	0.14506362	0.13309487	0.1450997	0.13313095
CAM-B3LYP // B3LYP/6-31G(d,p), vertical ΔSCF & CPCM	0.1096695	0.10699684	0.11360043	0.11092777	0.11368214	0.11100949
CAM-B3LYP // B3LYP/6-31G(d,p), orbital energies & CPCM	1.11474536	1.1213688	1.10459251	1.11121595	1.10471986	1.1113433
B3LYP // B3LYP/6-31G(d,p), adiabatic ΔSCF & ZPVC & CPCM	0.08178387	0.06051903	0.11353702	0.09227217	0.11318211	0.09191727
B3LYP // B3LYP/6-31G(d,p), adiabatic ΔSCF & CPCM	0.09934373	0.08737498	0.11184987	0.09988112	0.10637737	0.09440862
B3LYP // B3LYP/6-31G(d,p), vertical ΔSCF & CPCM	0.09749138	0.09481873	0.09591374	0.09324108	0.09048688	0.08781422
B3LYP // B3LYP/6-31G(d,p), orbital energies & CPCM	0.56865464	0.57527809	0.55815645	0.56477989	0.55793846	0.5645619
CAM-B3LYP // CAM-B3LYP/6-31G(d,p), adiabatic ΔSCF & ZPVC	0.23685022	0.24467919	0.19168667	0.19951564	0.19152597	0.19935494
CAM-B3LYP // CAM-B3LYP/6-31G(d,p), adiabatic ΔSCF	0.23282618	0.24031631	0.19245983	0.19994995	0.19774416	0.20523429
CAM-B3LYP // CAM-B3LYP/6-31G(d,p), vertical ΔSCF	0.23029964	0.23745092	0.18956725	0.19671853	0.1951334	0.20228468
CAM-B3LYP // CAM-B3LYP/6-31G(d,p), orbital energies	1.19022451	1.19703694	1.14396285	1.15077529	1.14464758	1.15146002
CAM-B3LYP // B3LYP/6-31G(d,p), adiabatic ΔSCF & ZPVC	0.23600827	0.24383724	0.19049938	0.19832835	0.18999333	0.1978223
CAM-B3LYP // B3LYP/6-31G(d,p), adiabatic ΔSCF	0.23988756	0.24737769	0.19401264	0.20150276	0.1937884	0.20127852
CAM-B3LYP // B3LYP/6-31G(d,p), vertical ΔSCF	0.21422198	0.22137326	0.16798102	0.1751323	0.16803859	0.17518987
CAM-B3LYP // B3LYP/6-31G(d,p), orbital energies	1.17924264	1.18605508	1.13263565	1.13944808	1.13297503	1.13978746
B3LYP // B3LYP/6-31G(d,p), adiabatic ΔSCF & ZPVC	0.25172308	0.25955204	0.20586884	0.21369781	0.20501745	0.21284642
B3LYP // B3LYP/6-31G(d,p), adiabatic ΔSCF	0.25299664	0.26048676	0.20161314	0.20910326	0.19588033	0.20337045
B3LYP // B3LYP/6-31G(d,p), vertical ΔSCF	0.30975243	0.31690371	0.2580029	0.26515418	0.2525519	0.25970318
B3LYP // B3LYP/6-31G(d,p), orbital energies	0.64493579	0.65174823	0.59798345	0.60479589	0.5979775	0.60478993

Table S4. Figures of merit for electron affinity for triple-zeta basis sets

(a) Slope (experimental ~ calculated)

	6-311G(d)	6-311G(d,p)	6-311+G(d)	6-311+G(d,p)	6-311++G(d)	6-311++G(d,p)
CAM-B3LYP // CAM-B3LYP/6-31G(d,p), adiabatic ΔSCF & ZPVC & CPCM	-0.215833	-0.2161816	-0.2271378	-0.2274864	-0.2282252	-0.2285737
CAM-B3LYP // CAM-B3LYP/6-31G(d,p), adiabatic ΔSCF & CPCM	-0.2465394	-0.244719	-0.2573699	-0.2555495	-0.2564103	-0.2545898
CAM-B3LYP // CAM-B3LYP/6-31G(d,p), vertical ΔSCF & CPCM	-0.1897599	-0.1867345	-0.1904481	-0.1874227	-0.1901615	-0.1871361
CAM-B3LYP // CAM-B3LYP/6-31G(d,p), orbital energies & CPCM	-0.2849985	-0.2817323	-0.2930738	-0.2898077	-0.2933671	-0.290101
CAM-B3LYP // B3LYP/6-31G(d,p), adiabatic ΔSCF & ZPVC & CPCM	-0.2133712	-0.2137197	-0.2281746	-0.2285232	-0.2288419	-0.2291904
CAM-B3LYP // B3LYP/6-31G(d,p), adiabatic ΔSCF & CPCM	-0.2492219	-0.2474014	-0.264336	-0.2625155	-0.2637411	-0.2619207
CAM-B3LYP // B3LYP/6-31G(d,p), vertical ΔSCF & CPCM	-0.2136141	-0.2105888	-0.2185859	-0.2155605	-0.2186641	-0.2156388
CAM-B3LYP // B3LYP/6-31G(d,p), orbital energies & CPCM	-0.3072126	-0.3039464	-0.3187866	-0.3155204	-0.3186598	-0.3153936
B3LYP // B3LYP/6-31G(d,p), adiabatic ΔSCF & ZPVC & CPCM	-0.3137364	-0.3140849	-0.3320385	-0.3323871	-0.3322857	-0.3326343
B3LYP // B3LYP/6-31G(d,p), adiabatic ΔSCF & CPCM	-0.3407607	-0.3389402	-0.3601583	-0.3583379	-0.3599283	-0.3581078

B3LYP // B3LYP/6-31G(d,p), vertical ΔSCF & CPCM	-0.3091375	-0.3061122	-0.3183928	-0.3153675	-0.3188359	-0.3158105
B3LYP // B3LYP/6-31G(d,p), orbital energies & CPCM	-0.3551592	-0.3518931	-0.3702319	-0.3669657	-0.369685	-0.3664189
CAM-B3LYP // CAM-B3LYP/6-31G(d,p), adiabatic ΔSCF & ZPVC	-0.4005705	-0.3991653	-0.4052809	-0.4038757	-0.4045901	-0.4031848
CAM-B3LYP // CAM-B3LYP/6-31G(d,p), adiabatic ΔSCF	-0.4274002	-0.4249952	-0.4304159	-0.4280108	-0.4302737	-0.4278687
CAM-B3LYP // CAM-B3LYP/6-31G(d,p), vertical ΔSCF	-0.5578539	-0.5554132	-0.5455914	-0.5431506	-0.5448027	-0.5423619
CAM-B3LYP // CAM-B3LYP/6-31G(d,p), orbital energies	-0.5800124	-0.5785	-0.5719589	-0.5704465	-0.5723881	-0.5708757
CAM-B3LYP // B3LYP/6-31G(d,p), adiabatic ΔSCF & ZPVC	-0.4021492	-0.400744	-0.4077237	-0.4063185	-0.4065771	-0.4051718
CAM-B3LYP // B3LYP/6-31G(d,p), adiabatic ΔSCF	-0.429293	-0.4268879	-0.4339576	-0.4315525	-0.4341446	-0.4317395
CAM-B3LYP // B3LYP/6-31G(d,p), vertical ΔSCF	-0.563941	-0.5615003	-0.5533275	-0.5508867	-0.5528679	-0.5504271
CAM-B3LYP // B3LYP/6-31G(d,p), orbital energies	-0.5873435	-0.5858311	-0.580154	-0.5786416	-0.5801274	-0.5786151
B3LYP // B3LYP/6-31G(d,p), adiabatic ΔSCF & ZPVC	-0.4611844	-0.4597791	-0.4676229	-0.4662177	-0.4660205	-0.4646153
B3LYP // B3LYP/6-31G(d,p), adiabatic ΔSCF	-0.4828238	-0.4804187	-0.4891374	-0.4867323	-0.4896535	-0.4872484
B3LYP // B3LYP/6-31G(d,p), vertical ΔSCF	-0.584959	-0.5825183	-0.5759945	-0.5735537	-0.575864	-0.5734232
B3LYP // B3LYP/6-31G(d,p), orbital energies	-0.6020297	-0.6005174	-0.5957043	-0.594192	-0.595222	-0.5937096

(b) Intercept (experimental ~ calculated)

	6-311G(d)	6-311G(d,p)	6-311+G(d)	6-311+G(d,p)	6-311++G(d)	6-311++G(d,p)
CAM-B3LYP // CAM-B3LYP/6-31G(d,p), adiabatic ΔSCF & ZPVC & CPCM	0.9529337	0.9529337	0.885105	0.885105	0.8870365	0.8870365
CAM-B3LYP // CAM-B3LYP/6-31G(d,p), adiabatic ΔSCF & CPCM	1.1327282	1.1327282	1.060313	1.060313	1.0629562	1.0629562
CAM-B3LYP // CAM-B3LYP/6-31G(d,p), vertical ΔSCF & CPCM	2.6782149	2.6782149	2.5452671	2.5452671	2.5474808	2.5474808
CAM-B3LYP // CAM-B3LYP/6-31G(d,p), orbital energies & CPCM	4.1196694	4.1196694	4.0624559	4.0624559	4.0661294	4.0661294
CAM-B3LYP // B3LYP/6-31G(d,p), adiabatic ΔSCF & ZPVC & CPCM	0.9024153	0.9024153	0.8668208	0.8668208	0.8758789	0.8758789
CAM-B3LYP // B3LYP/6-31G(d,p), adiabatic ΔSCF & CPCM	1.1075607	1.1075607	1.0625935	1.0625935	1.0675769	1.0675769
CAM-B3LYP // B3LYP/6-31G(d,p), vertical ΔSCF & CPCM	2.6243573	2.6243573	2.5140713	2.5140713	2.5138391	2.5138391
CAM-B3LYP // B3LYP/6-31G(d,p), orbital energies & CPCM	4.0501947	4.0501947	4.0108566	4.0108566	4.007298	4.007298
B3LYP // B3LYP/6-31G(d,p), adiabatic ΔSCF & ZPVC & CPCM	1.245115	1.245115	1.2312739	1.2312739	1.2369778	1.2369778
B3LYP // B3LYP/6-31G(d,p), adiabatic ΔSCF & CPCM	1.4107411	1.4107411	1.3897282	1.3897282	1.3935584	1.3935584
B3LYP // B3LYP/6-31G(d,p), vertical ΔSCF & CPCM	2.7343349	2.7343349	2.6502041	2.6502041	2.6510197	2.6510197
B3LYP // B3LYP/6-31G(d,p), orbital energies & CPCM	2.2001629	2.2001629	2.1891811	2.1891811	2.1888711	2.1888711
CAM-B3LYP // CAM-B3LYP/6-31G(d,p), adiabatic ΔSCF & ZPVC	3.6481483	3.6481483	3.5493876	3.5493876	3.54417	3.54417
CAM-B3LYP // CAM-B3LYP/6-31G(d,p), adiabatic ΔSCF	3.7148541	3.7148541	3.6138954	3.6138954	3.6103968	3.6103968
CAM-B3LYP // CAM-B3LYP/6-31G(d,p), vertical ΔSCF	3.9609574	3.9609574	3.878222	3.878222	3.8768119	3.8768119
CAM-B3LYP // CAM-B3LYP/6-31G(d,p), orbital energies	4.0631677	4.0631677	4.0197764	4.0197764	4.0203083	4.0203083
CAM-B3LYP // B3LYP/6-31G(d,p), adiabatic ΔSCF & ZPVC	3.6505737	3.6505737	3.5529198	3.5529198	3.544313	3.544313
CAM-B3LYP // B3LYP/6-31G(d,p), adiabatic ΔSCF	3.7147947	3.7147947	3.6171438	3.6171438	3.6124569	3.6124569
CAM-B3LYP // B3LYP/6-31G(d,p), vertical ΔSCF	3.9088615	3.9088615	3.8316347	3.8316347	3.8312374	3.8312374

CAM-B3LYP // B3LYP/6-31G(d,p), orbital energies	4.0219963	4.0219963	3.9863146	3.9863146	3.9900602	3.9900602
B3LYP // B3LYP/6-31G(d,p), adiabatic ΔSCF & ZPVC	3.5988947	3.5988947	3.5128284	3.5128284	3.5113131	3.5113131
B3LYP // B3LYP/6-31G(d,p), adiabatic ΔSCF	3.6632806	3.6632806	3.572431	3.572431	3.5700495	3.5700495
B3LYP // B3LYP/6-31G(d,p), vertical ΔSCF	3.879143	3.879143	3.8039313	3.8039313	3.8010531	3.8010531
B3LYP // B3LYP/6-31G(d,p), orbital energies	2.8641193	2.8641193	2.8256666	2.8256666	2.822145	2.822145

(c) R^2(experimental ~ calculated)

	6-311G(d)	6-311G(d,p)	6-311+G(d)	6-311+G(d,p)	6-311++G(d)	6-311++G(d,p)
CAM-B3LYP // CAM-B3LYP/6-31G(d,p), adiabatic ΔSCF & ZPVC & CPCM	-0.1497302	-0.1506531	-0.131926	-0.1328489	-0.1347751	-0.1356981
CAM-B3LYP // CAM-B3LYP/6-31G(d,p), adiabatic ΔSCF & CPCM	-0.1501546	-0.1504622	-0.132887	-0.1331947	-0.1329024	-0.1332101
CAM-B3LYP // CAM-B3LYP/6-31G(d,p), vertical ΔSCF & CPCM	-0.1608752	-0.1605675	-0.1374767	-0.137169	-0.1384171	-0.1381094
CAM-B3LYP // CAM-B3LYP/6-31G(d,p), orbital energies & CPCM	-0.1472796	-0.1463567	-0.1356745	-0.1347515	-0.1369064	-0.1359834
CAM-B3LYP // B3LYP/6-31G(d,p), adiabatic ΔSCF & ZPVC & CPCM	-0.1537404	-0.1546634	-0.1355653	-0.1364883	-0.1356977	-0.1366206
CAM-B3LYP // B3LYP/6-31G(d,p), adiabatic ΔSCF & CPCM	-0.1510932	-0.1514008	-0.1352217	-0.1355293	-0.1342872	-0.1345949
CAM-B3LYP // B3LYP/6-31G(d,p), vertical ΔSCF & CPCM	-0.155762	-0.1554544	-0.1345974	-0.1342898	-0.1354258	-0.1351181
CAM-B3LYP // B3LYP/6-31G(d,p), orbital energies & CPCM	-0.1422634	-0.1413404	-0.1328009	-0.1318779	-0.1338295	-0.1329065
B3LYP // B3LYP/6-31G(d,p), adiabatic ΔSCF & ZPVC & CPCM	-0.1405859	-0.1415089	-0.1275081	-0.1284311	-0.1303919	-0.1313148
B3LYP // B3LYP/6-31G(d,p), adiabatic ΔSCF & CPCM	-0.1376531	-0.1379607	-0.1269701	-0.1272778	-0.1288783	-0.129186
B3LYP // B3LYP/6-31G(d,p), vertical ΔSCF & CPCM	-0.1491664	-0.1488587	-0.1323525	-0.1320448	-0.1351857	-0.134878
B3LYP // B3LYP/6-31G(d,p), orbital energies & CPCM	-0.1294166	-0.1284936	-0.1225379	-0.1216149	-0.1238044	-0.1228814
CAM-B3LYP // CAM-B3LYP/6-31G(d,p), adiabatic ΔSCF & ZPVC	-0.1661868	-0.1671098	-0.1499834	-0.1509063	-0.1513896	-0.1523125
CAM-B3LYP // CAM-B3LYP/6-31G(d,p), adiabatic ΔSCF	-0.1690478	-0.1693554	-0.1514877	-0.1517954	-0.1533778	-0.1536855
CAM-B3LYP // CAM-B3LYP/6-31G(d,p), vertical ΔSCF	-0.312907	-0.3125994	-0.2817267	-0.2814191	-0.2822634	-0.2819558
CAM-B3LYP // CAM-B3LYP/6-31G(d,p), orbital energies	-0.2878764	-0.2869534	-0.2637982	-0.2628752	-0.265146	-0.264223
CAM-B3LYP // B3LYP/6-31G(d,p), adiabatic ΔSCF & ZPVC	-0.1736203	-0.1745433	-0.1559907	-0.1569136	-0.1536247	-0.1545477
CAM-B3LYP // B3LYP/6-31G(d,p), adiabatic ΔSCF	-0.1744118	-0.1747195	-0.1571925	-0.1575001	-0.1570773	-0.157385
CAM-B3LYP // B3LYP/6-31G(d,p), vertical ΔSCF	-0.3045633	-0.3042557	-0.2745616	-0.2742539	-0.2739309	-0.2736232
CAM-B3LYP // B3LYP/6-31G(d,p), orbital energies	-0.2793916	-0.2784686	-0.2564006	-0.2554777	-0.2564898	-0.2555668
B3LYP // B3LYP/6-31G(d,p), adiabatic ΔSCF & ZPVC	-0.1816163	-0.1825392	-0.1680286	-0.1689515	-0.1673587	-0.1682816
B3LYP // B3LYP/6-31G(d,p), adiabatic ΔSCF	-0.1809037	-0.1812114	-0.1678175	-0.1681252	-0.1694897	-0.1697973
B3LYP // B3LYP/6-31G(d,p), vertical ΔSCF	-0.2878026	-0.2874949	-0.2610961	-0.2607885	-0.2614149	-0.2611072
B3LYP // B3LYP/6-31G(d,p), orbital energies	-0.272189	-0.271266	-0.2507265	-0.2498035	-0.2499982	-0.2490752

(d) Computation time as on single CPU core

	6-311G(d)	6-311G(d,p)	6-311+G(d)	6-311+G(d,p)	6-311++G(d)	6-311++G(d,p)
CAM-B3LYP // CAM-B3LYP/6-31G(d,p), adiabatic ΔSCF & ZPVC & CPCM	9328.823	11062.934	25757.838	28727.715	30145.565	34351.21
CAM-B3LYP // CAM-B3LYP/6-31G(d,p), adiabatic ΔSCF & CPCM	8872.498	11313.267	26273.331	29721.96	29987.899	34444.39
CAM-B3LYP // CAM-B3LYP/6-31G(d,p), vertical ΔSCF & CPCM	9559.43	11676.136	25239.923	28136.582	29285.831	32962.44
CAM-B3LYP // CAM-B3LYP/6-31G(d,p), orbital energies & CPCM	3708.066	4469.989	10182.149	11496.119	10769.985	12636
CAM-B3LYP // B3LYP/6-31G(d,p), adiabatic ΔSCF & ZPVC & CPCM	9465.118	11199.229	25128.975	28098.853	29629.267	33834.91
CAM-B3LYP // B3LYP/6-31G(d,p), adiabatic ΔSCF & CPCM	8809.203	11249.972	25668.159	29116.787	29718.571	34175.06
CAM-B3LYP // B3LYP/6-31G(d,p), vertical ΔSCF & CPCM	9263.47	11380.176	24625.365	27522.025	29230.398	32907.01
CAM-B3LYP // B3LYP/6-31G(d,p), orbital energies & CPCM	3146.366	3908.289	9525.132	10839.101	10895.372	12761.39
B3LYP // B3LYP/6-31G(d,p), adiabatic ΔSCF & ZPVC & CPCM	8326.182	10060.293	21665.553	24635.43	24719.08	28924.72
B3LYP // B3LYP/6-31G(d,p), adiabatic ΔSCF & CPCM	6779.978	9220.746	21537.727	24986.355	24364.655	28821.14
B3LYP // B3LYP/6-31G(d,p), vertical ΔSCF & CPCM	7746.3	9863.006	21230.27	24126.929	24835.098	28511.71
B3LYP // B3LYP/6-31G(d,p), orbital energies & CPCM	3543.597	4305.52	8267.716	9581.686	8861.032	10727.05
CAM-B3LYP // CAM-B3LYP/6-31G(d,p), adiabatic ΔSCF & ZPVC	9328.823	11062.934	25757.838	28727.715	30145.565	34351.21
CAM-B3LYP // CAM-B3LYP/6-31G(d,p), adiabatic ΔSCF	8872.498	11313.267	26273.331	29721.96	29987.899	34444.39
CAM-B3LYP // CAM-B3LYP/6-31G(d,p), vertical ΔSCF	9559.43	11676.136	25239.923	28136.582	29285.831	32962.44
CAM-B3LYP // CAM-B3LYP/6-31G(d,p), orbital energies	3708.066	4469.989	10182.149	11496.119	10769.985	12636
CAM-B3LYP // B3LYP/6-31G(d,p), adiabatic ΔSCF & ZPVC	9465.118	11199.229	25128.975	28098.853	29629.267	33834.91
CAM-B3LYP // B3LYP/6-31G(d,p), adiabatic ΔSCF	8809.203	11249.972	25668.159	29116.787	29718.571	34175.06
CAM-B3LYP // B3LYP/6-31G(d,p), vertical ΔSCF	9263.47	11380.176	24625.365	27522.025	29230.398	32907.01
CAM-B3LYP // B3LYP/6-31G(d,p), orbital energies	3146.366	3908.289	9525.132	10839.101	10895.372	12761.39
B3LYP // B3LYP/6-31G(d,p), adiabatic ΔSCF & ZPVC	8326.182	10060.293	21665.553	24635.43	24719.08	28924.72
B3LYP // B3LYP/6-31G(d,p), adiabatic ΔSCF	6779.978	9220.746	21537.727	24986.355	24364.655	28821.14
B3LYP // B3LYP/6-31G(d,p), vertical ΔSCF	7746.3	9863.006	21230.27	24126.929	24835.098	28511.71
B3LYP // B3LYP/6-31G(d,p), orbital energies	3543.597	4305.52	8267.716	9581.686	8861.032	10727.05

(e) Mean absolute deviations of results

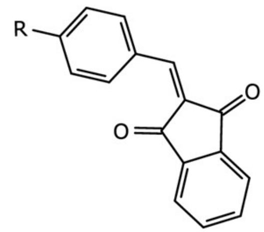
	6-311G(d)	6-311G(d,p)	6-311+G(d)	6-311+G(d,p)	6-311++G(d)	6-311++G(d,p)
CAM-B3LYP // CAM-B3LYP/6-31G(d,p), adiabatic ΔSCF & ZPVC & CPCM	0.13616709	0.14797859	0.0537274	0.0655389	0.04765984	0.05947134
CAM-B3LYP // CAM-B3LYP/6-31G(d,p), adiabatic ΔSCF & CPCM	0.22447184	0.23628334	0.10043764	0.11224914	0.11032289	0.12213439
CAM-B3LYP // CAM-B3LYP/6-31G(d,p), vertical ΔSCF & CPCM	2.38717527	2.39898678	2.22844052	2.24025202	2.23797239	2.24978389
CAM-B3LYP // CAM-B3LYP/6-31G(d,p), orbital energies & CPCM	4.21539795	4.22720945	4.14041531	4.15222681	4.1339502	4.1457617
CAM-B3LYP // B3LYP/6-31G(d,p), adiabatic ΔSCF & ZPVC & CPCM	0.09847235	0.11028385	0.06612636	0.07793786	0.06109213	0.07290363
CAM-B3LYP // B3LYP/6-31G(d,p), adiabatic ΔSCF & CPCM	0.17771277	0.18952427	0.0773318	0.0891433	0.07677516	0.08858666
CAM-B3LYP // B3LYP/6-31G(d,p), vertical ΔSCF & CPCM	2.28131521	2.29312671	2.13121648	2.14302798	2.13025451	2.14206601

CAM-B3LYP // B3LYP/6-31G(d,p), orbital energies & CPCM	4.13573043	4.14754193	4.06578989	4.07760139	4.06020225	4.07201375
B3LYP // B3LYP/6-31G(d,p), adiabatic ΔSCF & ZPVC & CPCM	0.06998387	0.08179537	0.09752479	0.10933629	0.10331709	0.11512859
B3LYP // B3LYP/6-31G(d,p), adiabatic ΔSCF & CPCM	0.13481675	0.14662825	0.06788221	0.07969371	0.06667687	0.07848837
B3LYP // B3LYP/6-31G(d,p), vertical ΔSCF & CPCM	2.21643004	2.22824154	2.08476055	2.09657205	2.08309792	2.09490942
B3LYP // B3LYP/6-31G(d,p), orbital energies & CPCM	1.25207448	1.26388598	1.19696924	1.20878074	1.20205227	1.21386377
CAM-B3LYP // CAM-B3LYP/6-31G(d,p), adiabatic ΔSCF & ZPVC	3.49415569	3.50596719	3.31532668	3.32713818	3.31288847	3.32469997
CAM-B3LYP // CAM-B3LYP/6-31G(d,p), adiabatic ΔSCF	3.58380465	3.59561615	3.40399422	3.41580572	3.40911748	3.42092898
CAM-B3LYP // CAM-B3LYP/6-31G(d,p), vertical ΔSCF	4.06188064	4.07369214	3.86918359	3.88099509	3.87430475	3.88611625
CAM-B3LYP // CAM-B3LYP/6-31G(d,p), orbital energies	4.31165261	4.32346411	4.20572245	4.21753395	4.20394052	4.21575202
CAM-B3LYP // B3LYP/6-31G(d,p), adiabatic ΔSCF & ZPVC	3.49818127	3.50999277	3.31642632	3.32823782	3.31034479	3.32215629
CAM-B3LYP // B3LYP/6-31G(d,p), adiabatic ΔSCF	3.59108228	3.60289378	3.40934179	3.42115329	3.40821719	3.42002869
CAM-B3LYP // B3LYP/6-31G(d,p), vertical ΔSCF	3.95497423	3.96678573	3.76398432	3.77579582	3.76289441	3.77470591
CAM-B3LYP // B3LYP/6-31G(d,p), orbital energies	4.22982446	4.24163596	4.13187998	4.14369148	4.1265651	4.1383766
B3LYP // B3LYP/6-31G(d,p), adiabatic ΔSCF & ZPVC	3.35965989	3.37147139	3.18477221	3.19658371	3.18484055	3.19665205
B3LYP // B3LYP/6-31G(d,p), adiabatic ΔSCF	3.45663315	3.46844465	3.28275579	3.29456729	3.28517654	3.29698804
B3LYP // B3LYP/6-31G(d,p), vertical ΔSCF	3.87474213	3.88655363	3.69525255	3.70706405	3.69774479	3.70955629
B3LYP // B3LYP/6-31G(d,p), orbital energies	1.34338596	1.35519746	1.26322034	1.27503184	1.26416573	1.27597723

Supplementary material 2B. Electrochemical redox potentials determined in cyclic voltammetry experiment

Measurements are taken in acetonitrile in presence of supporting electrolyte tetrabutylammonium tetrafluorophosphate ($TBAPF_6$) of concentration 0,1 M. Computer-controlled electrochemical system *PARSAT 2273* was used, with glassy carbon disk (Ø 0.5 cm) as a working electrode and Pt wire as an auxiliary electrode. Potential scan rate was 100 mV/s. Potentials are expressed relative to saturated calomel electrode (E° = + 0.2412 vs. standard hydrogen electrode in water).

Table S5. Electrochemical redox potentials determined in cyclic voltammetry experiments



Substitutient R	E_{ox}^{peak}	E_{red}^{peak}
OH	6.48	3.97
NMe_2	5.88	3.62
NH_2	5.99	3.64
NPh_2	6.01	3.78
[Julo]	5.7	3.6
NHCOCH_3	6.58	3.94
OCH_3	6.64	3.77
CH_3	6.98	3.82
H	7.06	3.86
F	7.14	3.88
Cl	-	3.95
COOCH_3	-	4.05
CN	-	4.13
NO_2	-	4.27
<u>Reference redox pair</u>		
Fc	0.22	

Supplementary material 3A. Popularity of computational methods for ionization

Web of Science™ was searched twice on dates mentioned below Search string was "ionization and *NNN*" where *NNN* is the corresponding method. There were also hits for "ionisation and *NNN*", not included in this study, though. Contamination of search results by non-chemical homonyms was hopefully reduced by adding "AND (COMPUT* OR CALCULAT*)" to the search string.
Most of various functionals were taken from DFT Popularity Poll 2015 (M. Swart, F. M. Bickelhaupt, M.Duran, Girona–Amsterdam, 2015)

Table S6. Results of *Web of Science*™ database search for computational methods popularity in the field of ionization and electron affinity

Method class	Hamiltonian	Hits 26.06.2015.	16.02.2016.	Comment
LDA	LDA		175	
LDA	SVWN	13	13	
GGA	hcth		0	
GGA	OLYP		4	
GGA	SOGGA	1	1	
GGA	PW91	39	41	
GGA	PBE	89	97	
GGA	BLYP	83	86	
GGA	BP86	57	60	
GGA	APBE		0	designed for asymptotic behaviour
GGA	LB94		17	designed for asymptotic behaviour
GGA+emp	S12g		0	
GGA+emp	optB88-vdW		0	also without dash (nothing found)
meta	M06-L	16	20	also without dash
meta	TPSS	16	21	
meta	revTPSS	0	0	
meta	tau-HCTH		0	
meta+emp	revTPSS-D		0	also without dash (nothing found)
meta+emp	SSB-D		0	also without dash (nothing found)
meta-nga	M11-L	1	1	also without dash (nothing found)
meta-nga	MN12-L	1	1	also without dash (nothing found)
GH	PBE0	92	99	in both cases also PBE1PBE
GH	O3LYP		8	
GH	B3LYP	2141	2224	
GH	B97X	23	27	
GH	B3PW91	68	72	

GH	BHandH		7	also BH&H
GH	BHandHLYP		28	also BH&HLYP
GH	mPW1k		9	
GH	B3LYP*		4	search(B3LYP*) - search(B3LYP)
GH	KMLYP		2	
GH	X3LYP		8	
GH+emp	S12h		0	
GH+emp	B3LYP-D	6	6	also without dash (nothing found)
GH+emp	B97-D	10	14	also without dash
GH-meta	TPSSh	6	7	
GH-meta	M08	4	5	
GH-meta	PW6B95		3	
GH-meta	M06-2X	62	84	also without dash
GH-meta	M06-HF	1	3	also without dash
GH-meta	M06	93	103	
GH-meta	M05-2X	25	33	also without dash
	Long-Range Correct*	128	137	
RSH	CAM-B3LYP	38	46	
RSH	LC-PBE	1	1	also without dash (nothing found)
RSH	LC-wPBE	0	0	also without dash (nothing found)
RSH	N12-SX	0	1	also without dash (nothing found)
RSH	wB97X	2	3	
RSH+emp	wB97X-D	2	5	also without dash
RSH-meta	M11	15	16	
RSH-meta-nga	MN12-SX	0	0	also without dash (nothing found)
scr-GH	HSE		7	WAS CONTAMINATED BY NON-CHEMISTRY
DH	B2PLYP	7	7	
DH+emp	DSD-BLYP	1	1	also without dash (nothing found)
DH+emp	DSD-PBEP86	0	0	also without dash (nothing found)
DH-meta	PWPB95-D3		1	with D*; also without dash (nothing found)
RPA	RPA	80	44	WAS CONTAMINATED BY NON-CHEMISTRY
orbital-dependent	SAOP	19	19	designed for asymptotic behaviour
WFT	HF		925	contaminated with hydrogen fluoride and hafnium
WFT	MP2	976	1004	

WFT	MP3	42	46	
WFT	MP4	60	60	
WFT	MP5	4	4	
WFT	CC2		46	not identical to CCSD
WFT	CCSD	584	611	
WFT	MCSCF	52	60	also with dash
WFT	CASSCF	273	282	also with dash
WFT	RASSCF	9	9	also with dash (nothing found)
EPT	OVGF	118	122	
EPT	EPT	11	11	

Legend:

LDA	Local Density Approximation
GGA	Generalized Gradient Approximation
meta	Functionals involving Laplacian of electron density
GH	Global hybrid functionals (same percentage of HF-like exchange in all spatial range)
DH	Double-hybrid functionals (involving perturbation theory and unoccupied orbitals)
emp	Empirical correction for DFT, mainly for dispersion interaction
RSH	Range-separated hybrid functionals (different percentage of HF-like exchange for close and distant electrons)
scr-GH	Screened global hybrid functional
RPA	Random phase approximation
WFT	Wave-function functional theory (classical *ab initio*)
EPT	Electron propagator theory

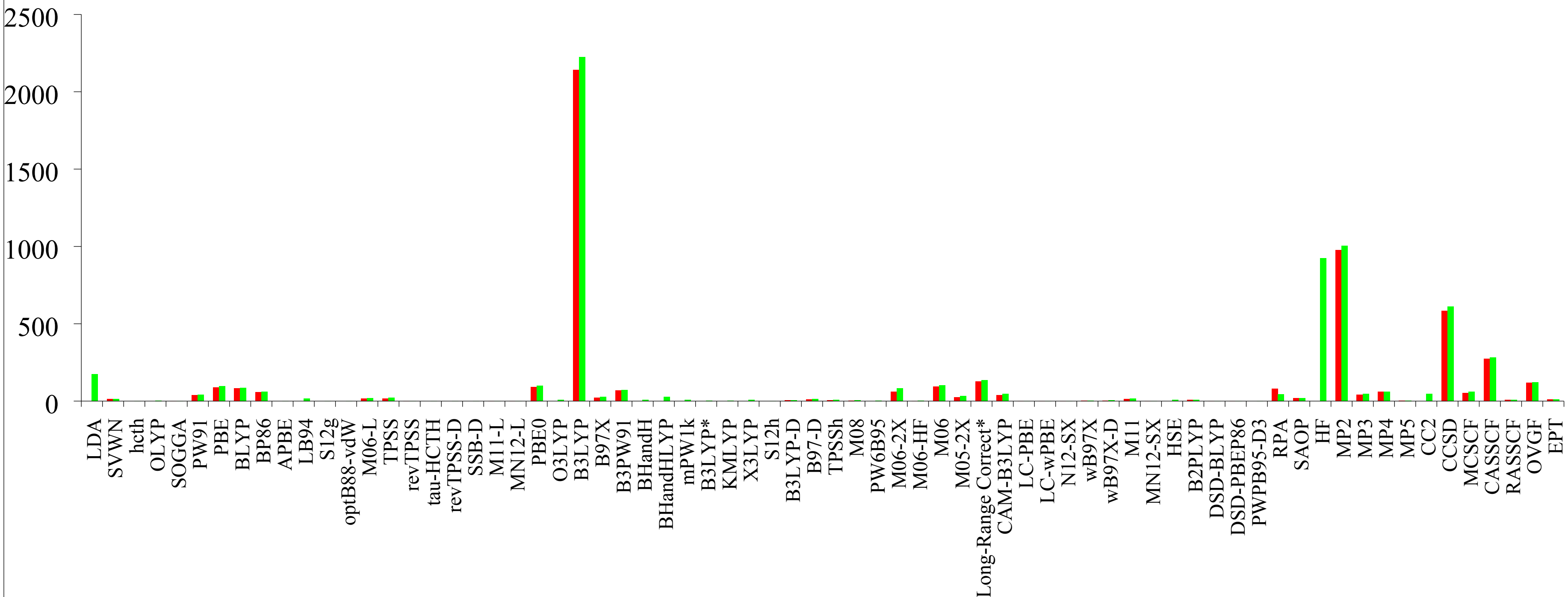


Figure S5. Popularity of various computational methods, from the search in *Web of Science*™

Supplementary material 3B. Popularity of terminology for ionization in the field of organic electronics

The search was conducted in middle 2014. All queries were entered in the "All fields" search category. Search string was formed as a combination from two terms: one characteristic to application, one describing the terminology; both were united by " AND " operator. As terminological term consisted of several expressions which were united by OR, it was put in parentheses.

Table S7. Results of scientific web database search for popularity of various terminologies in the field of ionization and electron affinity

Application term	Terminological term	Hits					
		Scopus™	*Web of Science™*	*Science Direct™*	*Scitation™*	*Wiley Online Library™*	*EBSCOhost Academic Search Complete™*
OLED	HOMO OR LUMO	1221	229	2311	7153	1454	194
photovoltaic	HOMO OR LUMO	4731	1225	5035	14304	3372	423
"solar cell"	HOMO OR LUMO	5946	532	5945	(20513)*	2898	192
OTFT	HOMO OR LUMO	84	39	250	590	182	24
OLED	"vertical ionization energy" OR "vertical ionization potential" OR "vertical electron affinity"	4	0	31	0	10	0
photovoltaic	"vertical ionization energy" OR "vertical ionization potential" OR "vertical electron affinity"	56	3	60	0	30	0
"solar cell"	"vertical ionization energy" OR "vertical ionization potential" OR "vertical electron affinity"	69	0	74	0	31	0
OTFT	"vertical ionization energy" OR "vertical ionization potential" OR "vertical electron affinity"	0	0	3	0	1	0
OLED	"adiabatic ionization energy" OR "adiabatic ionization potential" OR "adiabatic electron affinity"	5	1	23	0	4	1
photovoltaic	"adiabatic ionization energy" OR "adiabatic ionization potential" OR "adiabatic electron affinity"	17	3	47	0	18	0
"solar cell"	"adiabatic ionization energy" OR "adiabatic ionization potential" OR "adiabatic electron affinity"	51	0	49	0	19	0
OTFT	"adiabatic ionization energy" OR "adiabatic ionization potential" OR "adiabatic electron affinity"	1	0	3	0	1	0

* search error; result shown is for "solar AND cell", definitely contaminated

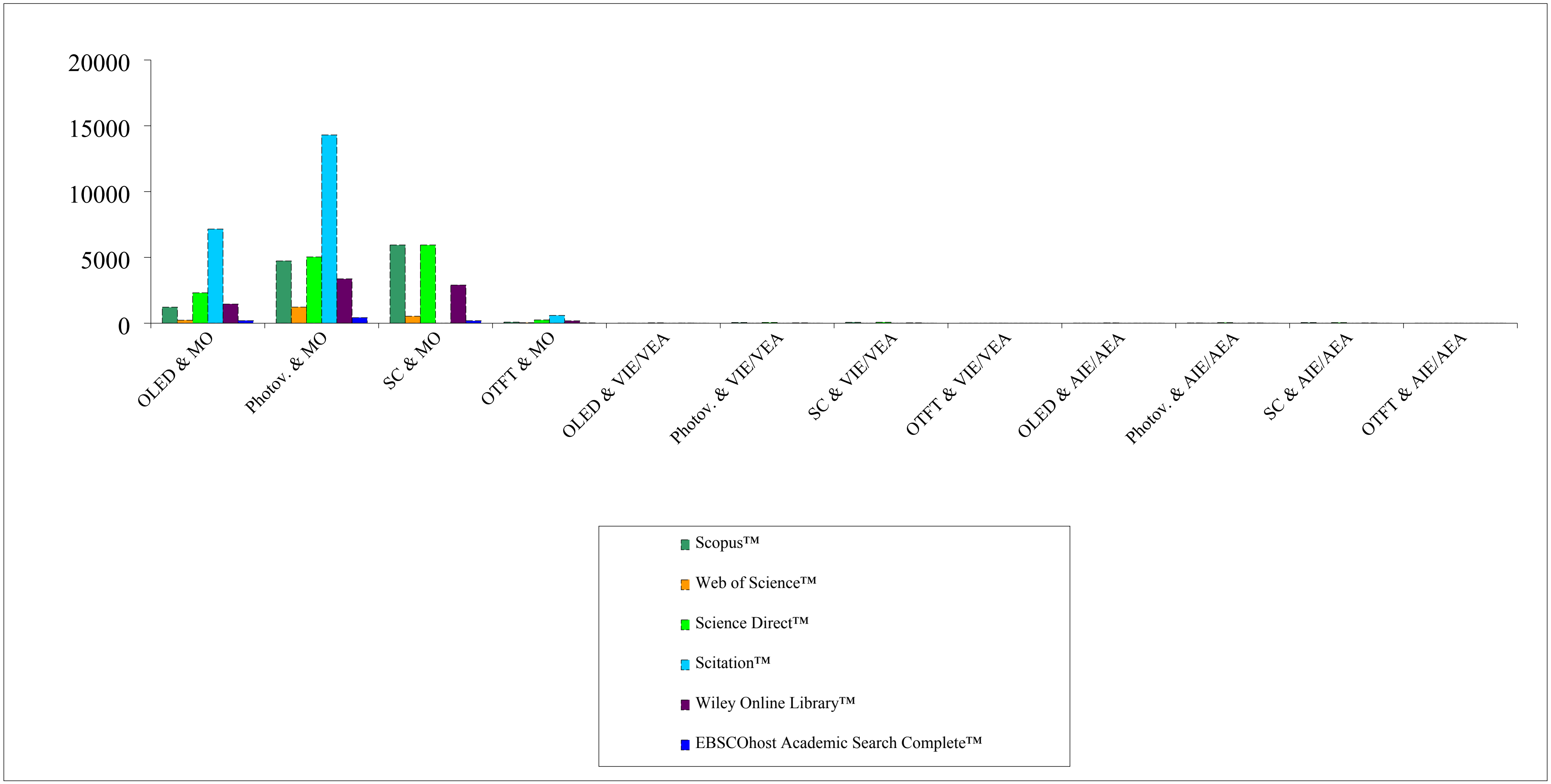


Figure S6. Popularity of different terminology in the field of organic electronics, from the search in *Web of Science*™