Modern battery electrolytes: Ion-ion interactions in Li^+/Na^+ conductors from *ab initio* calculations
Electronic supplementary information

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$\Delta E_{d_{Li}}$ vs. $\Delta E_{d_{Na}}$

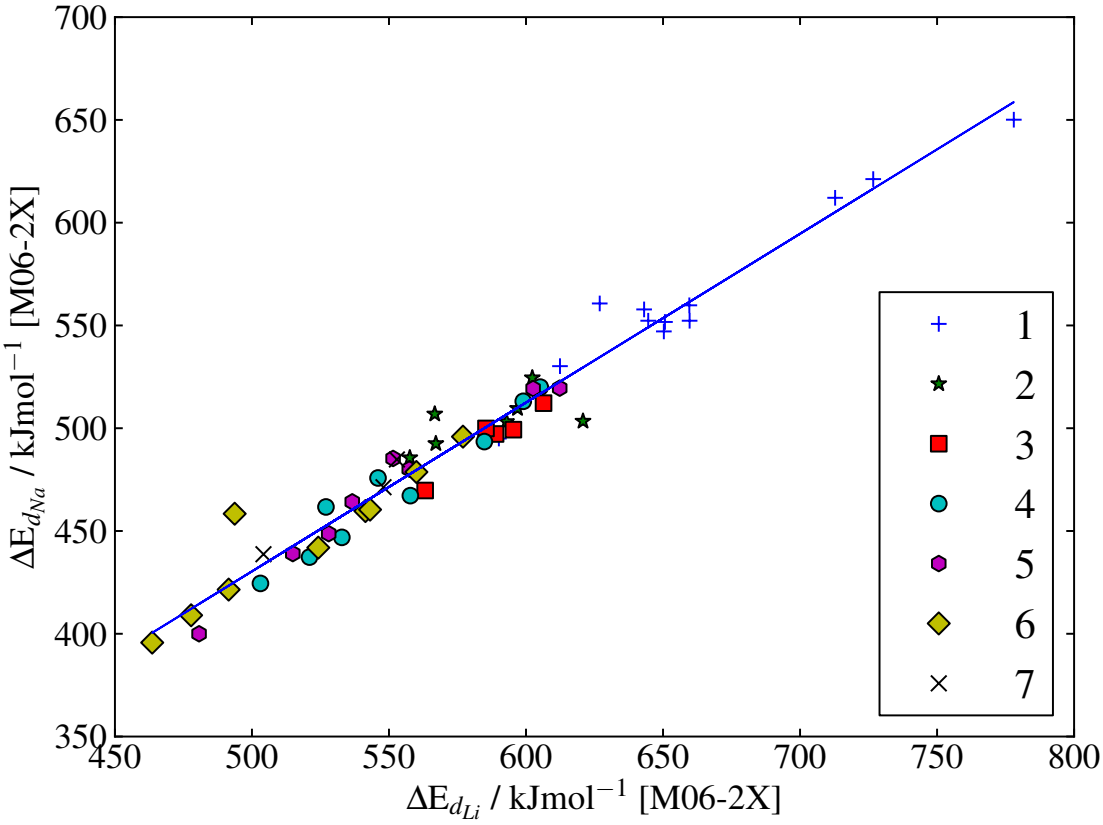


Figure 1: The ion-pair dissociation energies, $\Delta E_{d_{Li}}$ vs. $\Delta E_{d_{Na}}$, calculated with M06-2X/6-311+G* for the 53 anions. The numbers in the legend correspond to the grouping of the anions as described in the computational methodology section of the article.

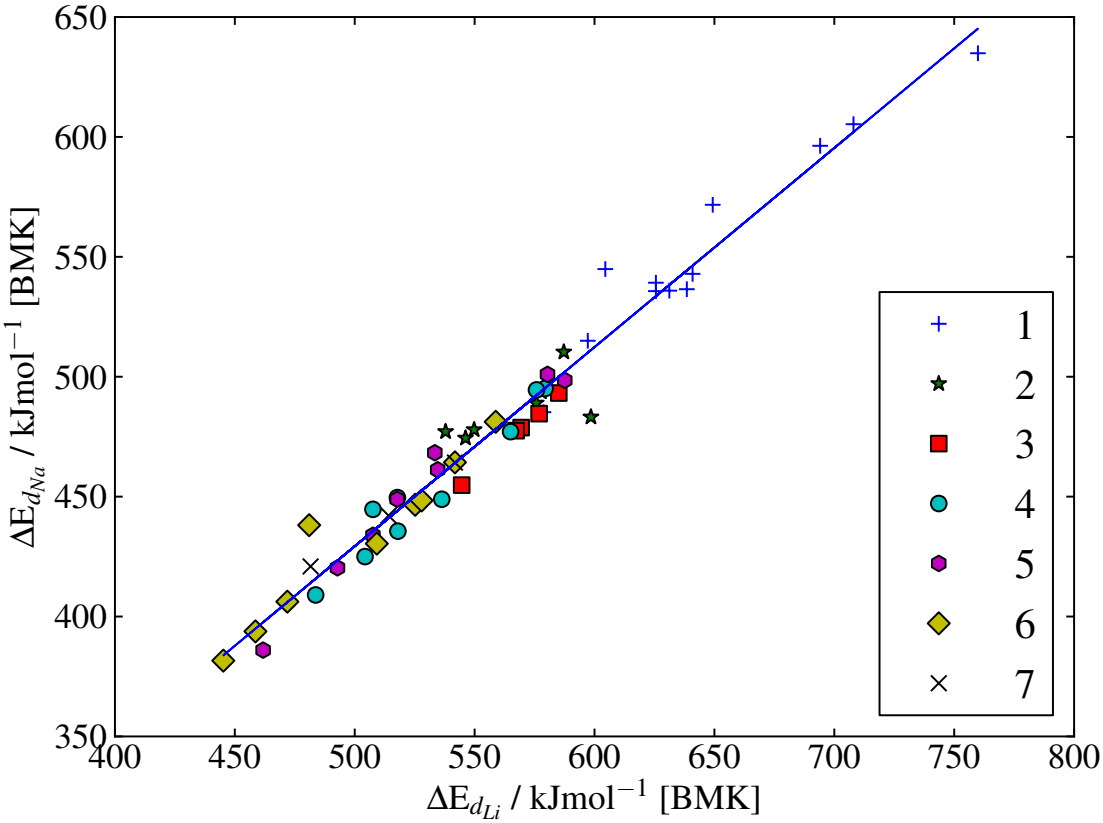


Figure 2: The ion-pair dissociation energies, $\Delta E_{d_{Li}}$ vs. $\Delta E_{d_{Na}}$, calculated with BMK/6-311+G* for the 53 anions. The numbers in the legend correspond to the grouping of the anions as described in the computational methodology section of the article.

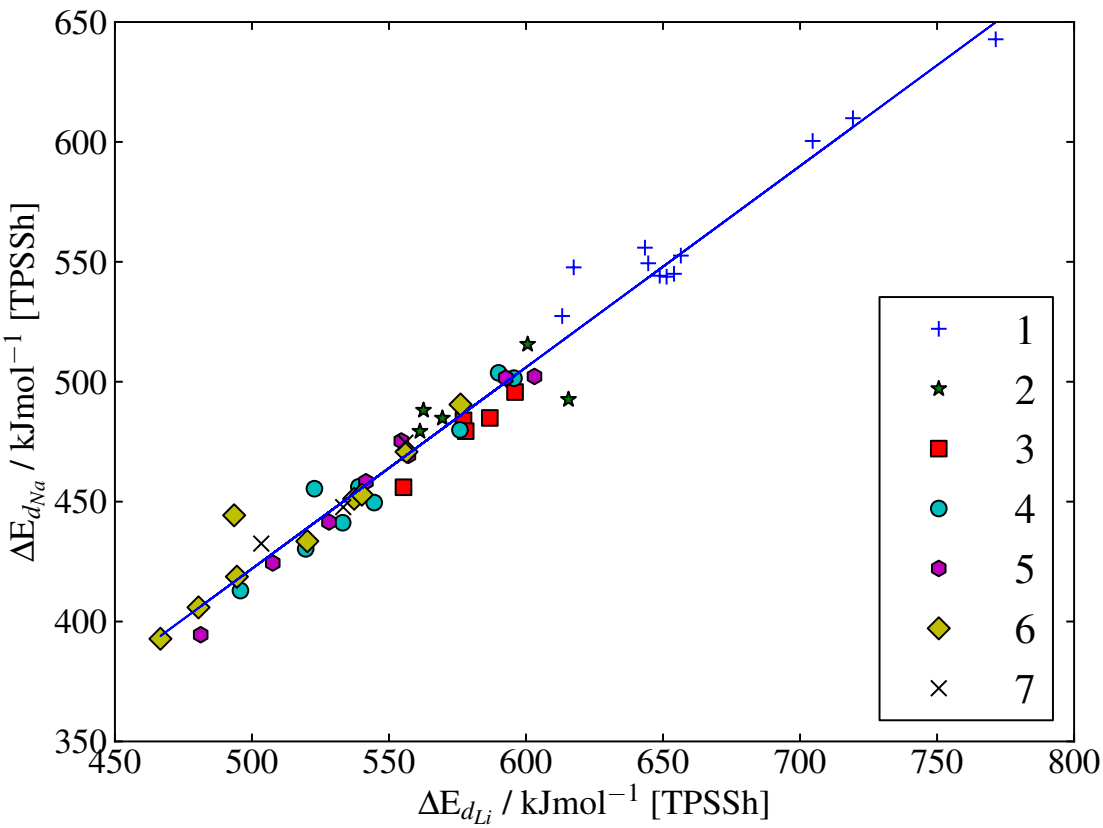
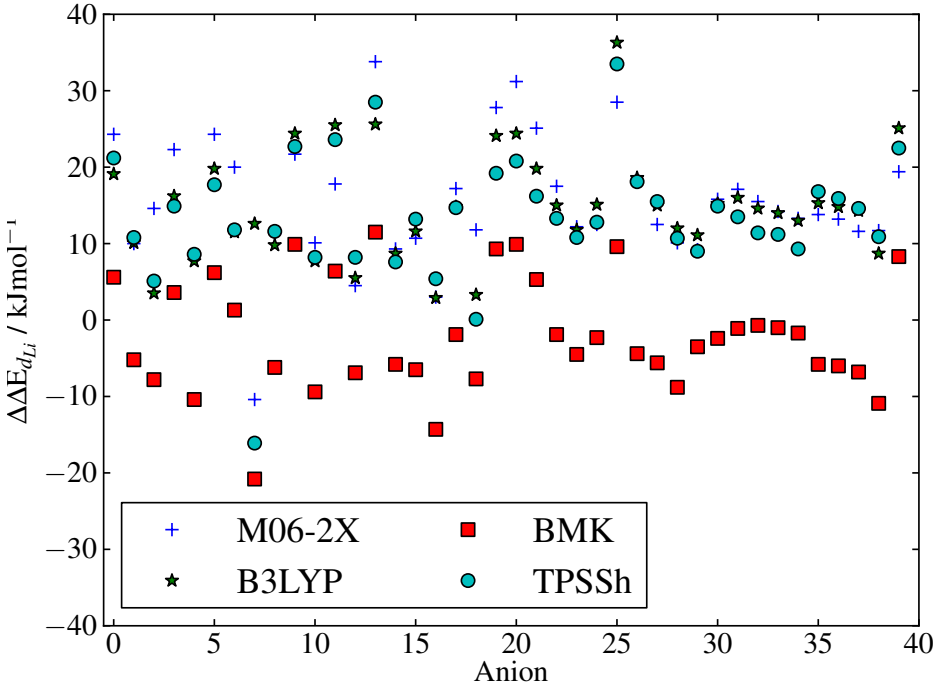
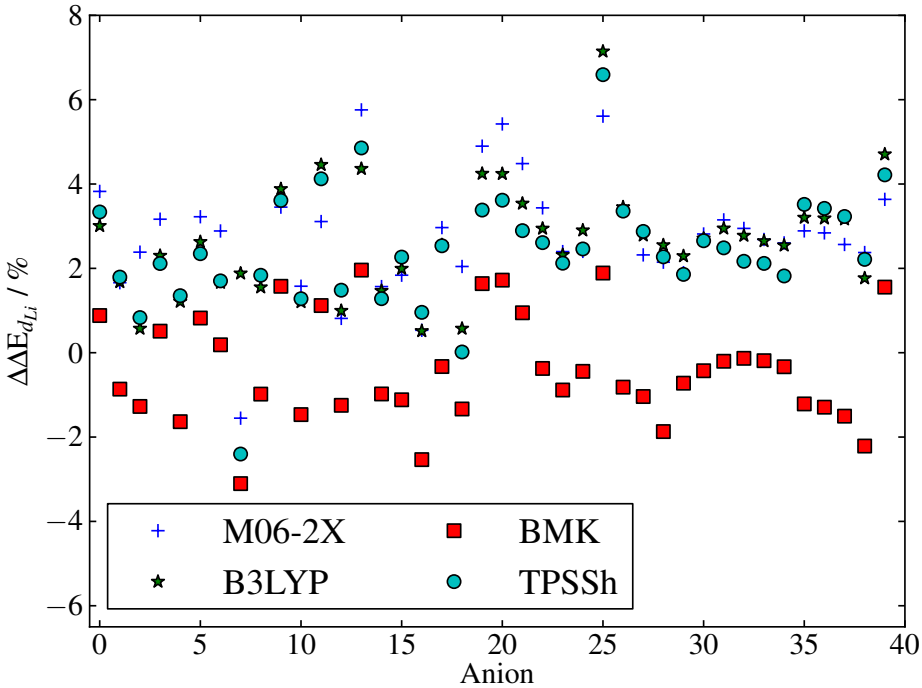


Figure 3: The ion-pair dissociation energies, $\Delta E_{d_{Li}}$ vs. $\Delta E_{d_{Na}}$, calculated with TPSSh/6-311+G* for the 53 anions. The numbers in the legend correspond to the grouping of the anions as described in the computational methodology section of the article.

Functional benchmarking

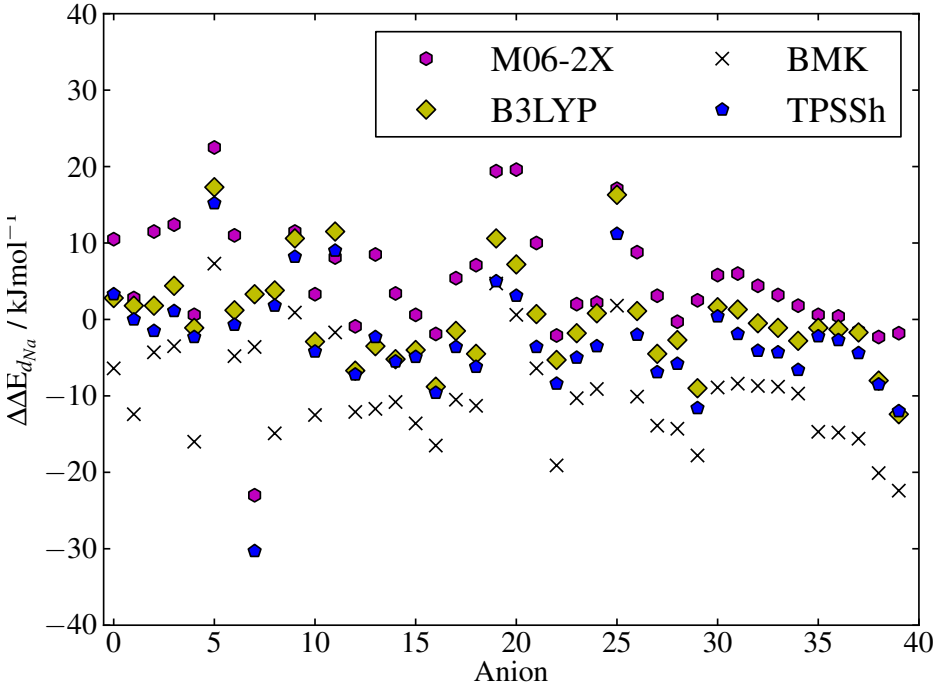


(a) Absolute deviation

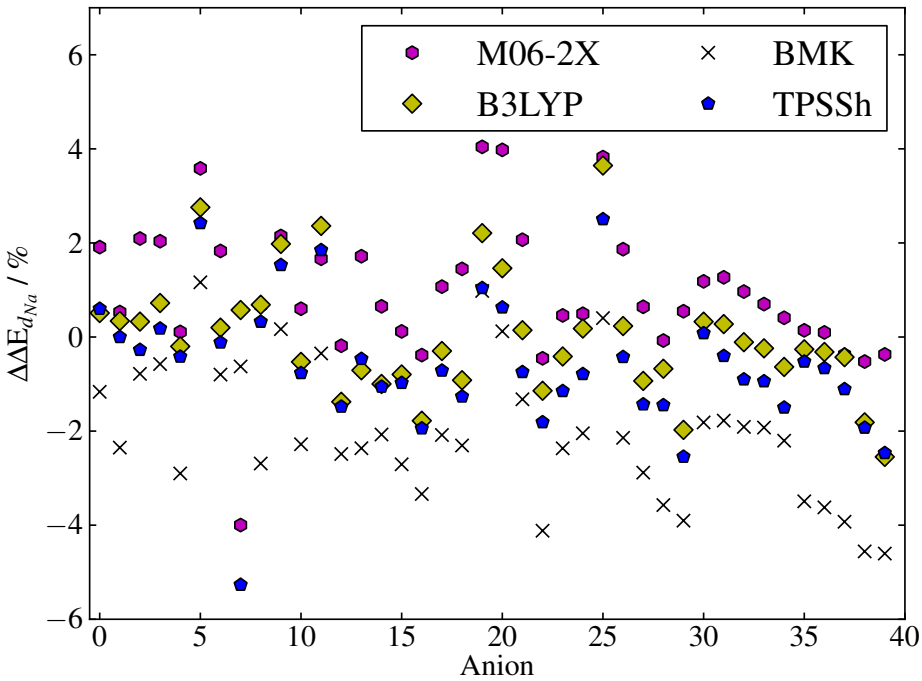


(b) Relative deviation

Figure 4: The deviation of the DFT functionals when benchmarked against the lithium ion-pair dissociation energy of G4MP2.



(a) Absolute deviation



(b) Relative deviation

Figure 5: The deviation of the DFT functionals when benchmarked against the sodium ion-pair dissociation energy of G4MP2.

Chemical structures