Assessment of the Density Functional Tight Binding Method for Protic Ionic Liquids

Supporting Information

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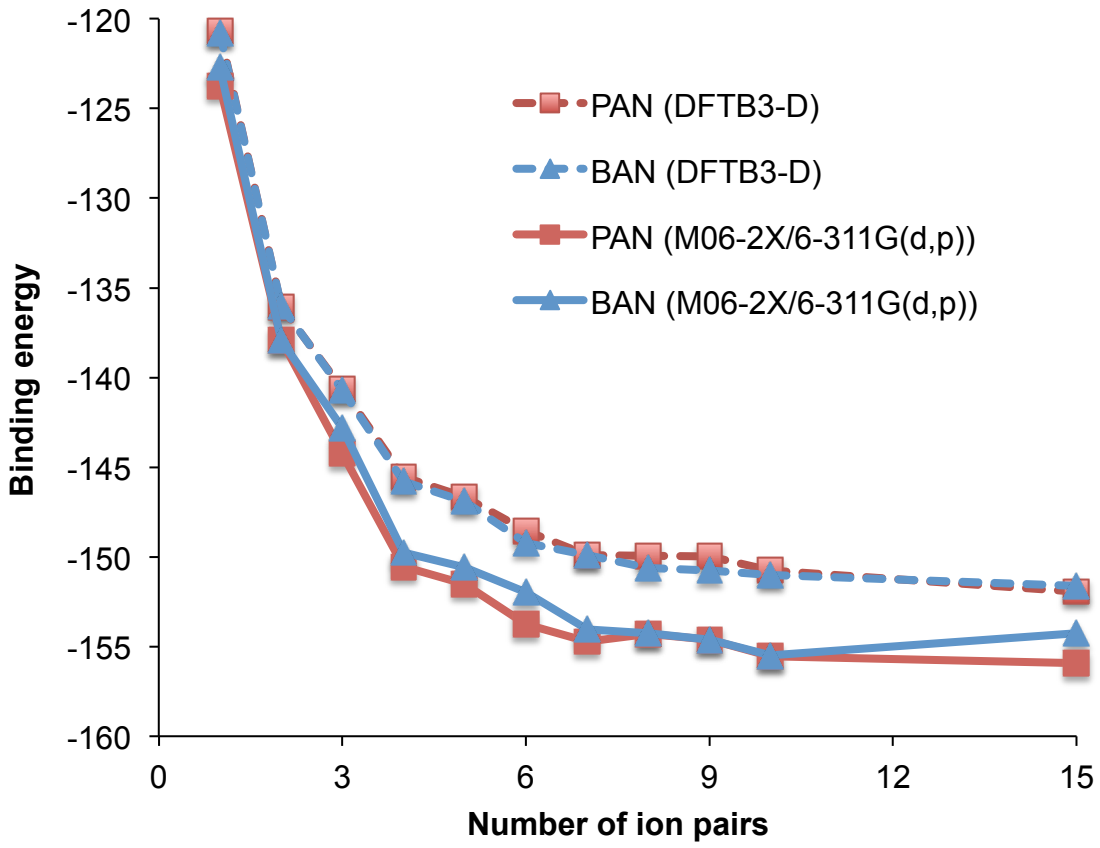

Figure S1. Comparison of binding energies (kcal/mol per ion pair) for propylammonium nitrate (PAN) and butyl ammonium nitrate (BAN) clusters, as a function of cluster size, computed with DFTB3-D and M06-2XS/6-311G(d,p).

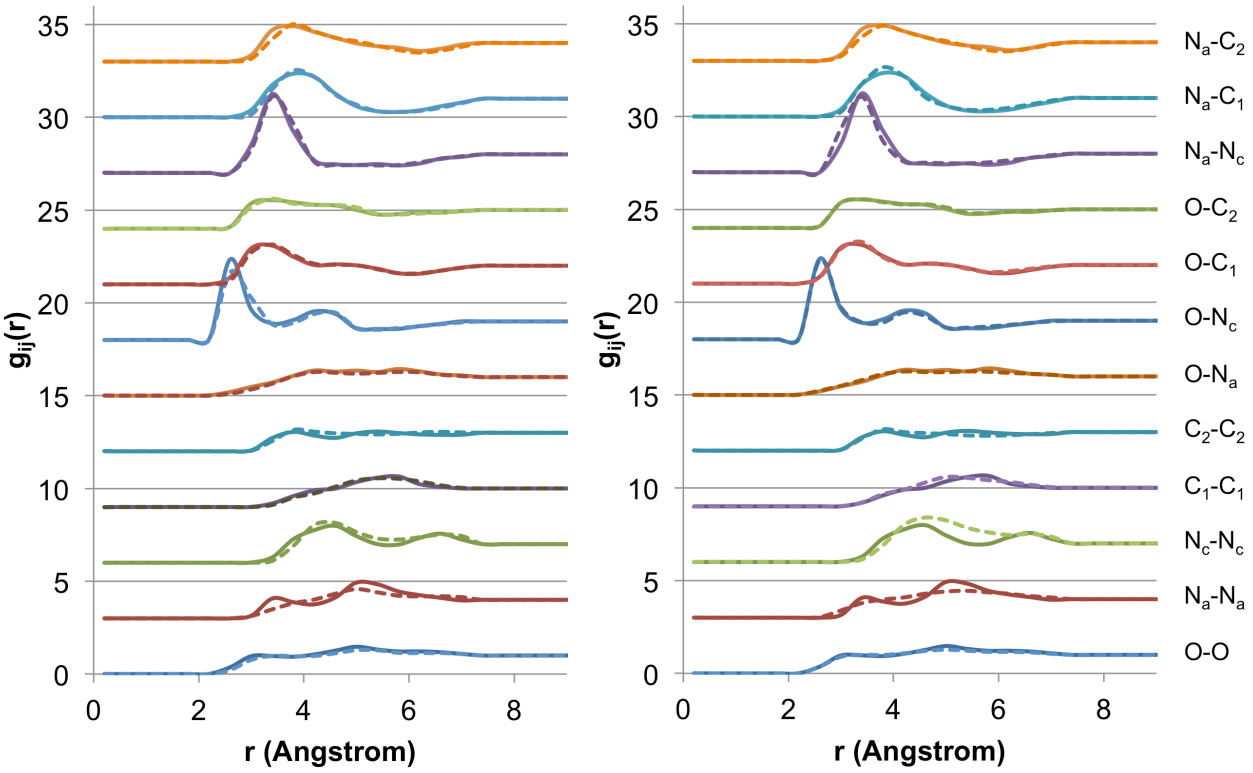

Figure S2. Comparison of simulated partial $g_{ij}(r)$ functions for bulk EAN (see Figure 5), simulated using (a) DFTB3-D/mio-0-1 (solid) and DFTB3-D/3ob-1-1 (dashed), and (b) DFTB3-D/mio-0-1 (solid) and DFTB2-D/mio-0-1 (dashed).

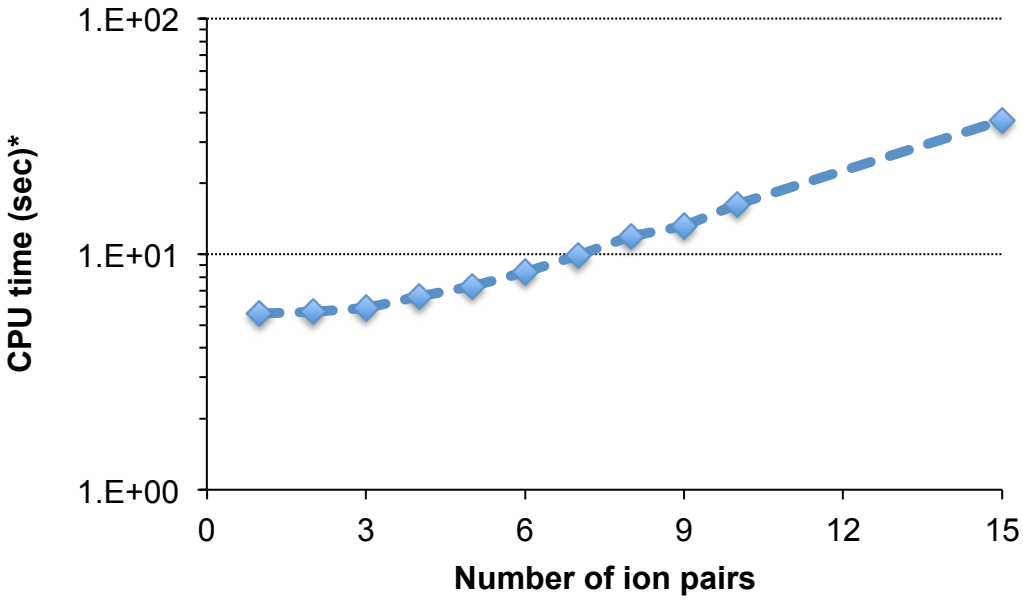

Figure S3. CPU time required for a single DFTB3-D/mio-0-1 energy and gradient calculation of EAN clusters, as a function of cluster size. These data were produced using an Intel hexacore Xeon E5-2667 2.9 GHz CPU and 2GB RAM. For reference, CPU times for equivalent DFT calculations

on these systems take ~1000 times longer, however for clusters > 6 ion pairs scaling is the same as for DFTB3-D/mio-0-1.