Towards large-scale, fully ab initio calculations of ionic liquids

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SUPPLEMENTARY INFORMATION
Figure S1. Walden plot for ionic liquids studied in ref. 11. Ionic liquids were grouped with respect to anions.
Figure S2. Born-Fajans-Haber cycle for calculating $\Delta_{\text{fus}} G^T$. 

\[ [A^+]_{\text{g}} + [X]_{\text{g}} \]

\[ + \Delta_{\text{lat}} G^T \]

\[ [A][X]_{(s)} \]

\[ \Delta_{\text{fus}} G^T \]

\[ [A][X]_{(l)} \]

\[ \Delta_{\text{solv}} G^T (A^+) \]

\[ \Delta_{\text{solv}} G^T (X^-) \]
Figure S3. Correlation between the proton affinity and melting point for C$_2$ mim-based ionic liquids incorporating anions: NTf$_2$, N(CN)$_2$, Cl, NO$_3$, CF$_3$SO$_3$ and (SO$_2$CH$_3$)N(SO$_2$CF$_3$).