ESI for:
A first-principles investigation of the structural and electrochemical properties of biredox ionic species in acetonitrile.

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1   Probabilities and Landau Free energies

We report here the probability distribution (left) and the Landau free energies (right). The symbols correspond to the data computed by molecular dynamics simulations while the dashed lines correspond to the TGS model with the parameters given in Table 2 of the main article.
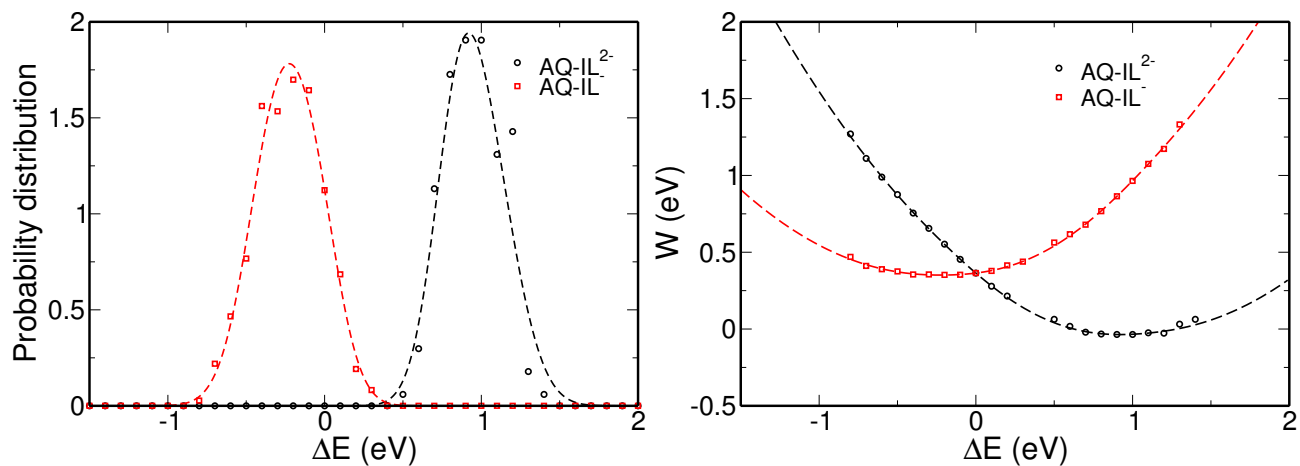

Figure S1 Probability distributions and Landau free energy curves for AQ-IL$^-$/AQ-IL^{2-}.
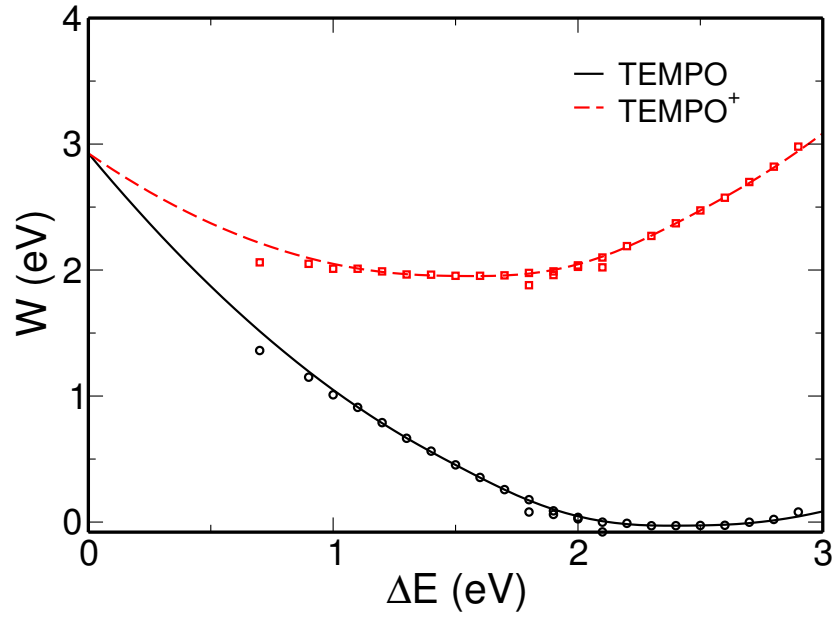
Figure S2 Landau free energy curves of TEMPO and TEMPO$^+$. The corresponding probability distribution is displayed in Figure 2 of the main article.
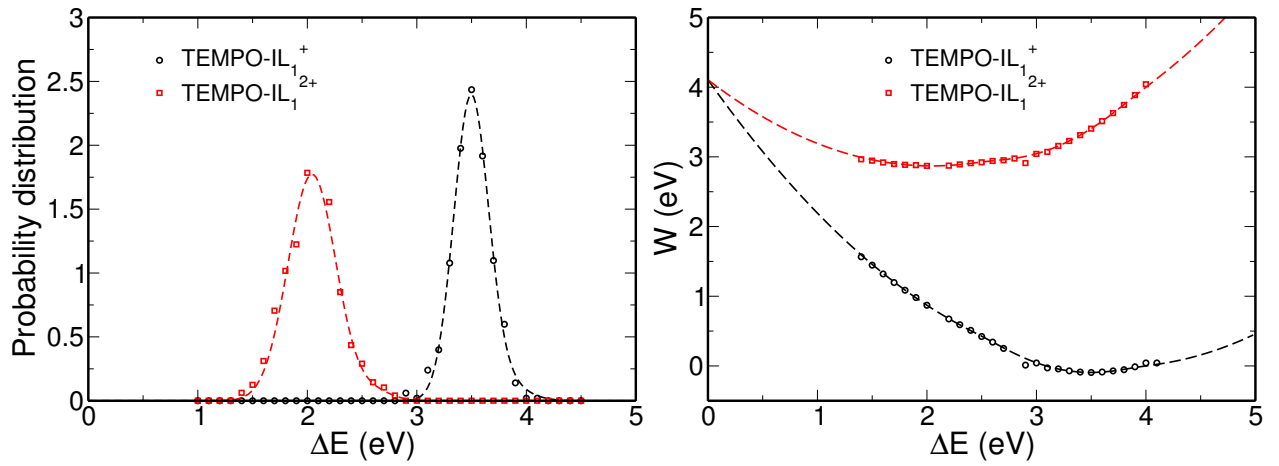

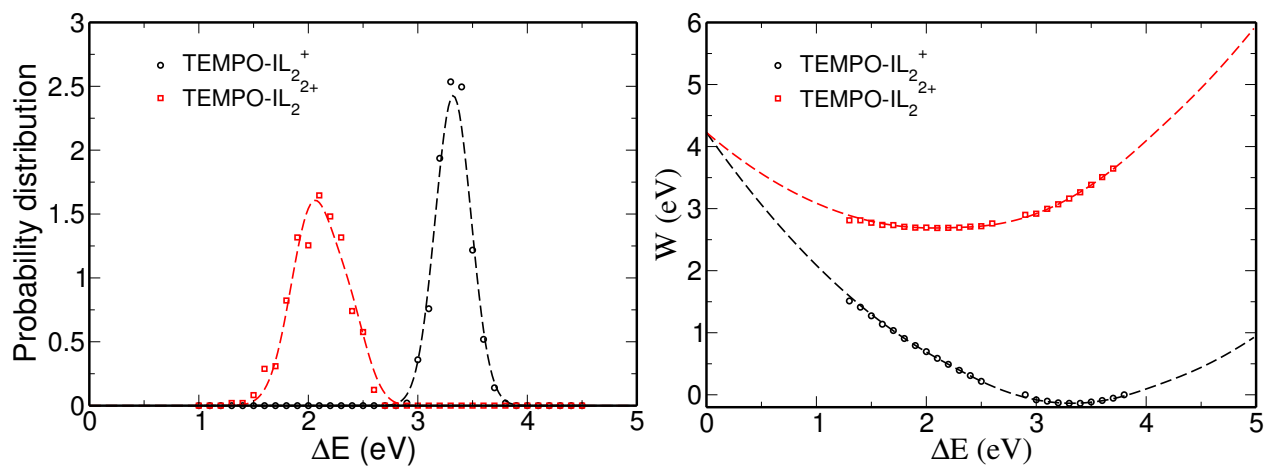Figure S3 Probability distributions and Landau free energy curves for TEMPO-IL_1^+/TEMPO-IL_1^{2+}.

Figure S4 Probability distributions and Landau free energy curves for TEMPO-IL$_2^+$/TEMPO-IL$_2^{2+}$.

2 Radial distribution functions

We report here the RDFs between selected acetonitrile atoms and the oxygen atoms from the ionic liquid moiety, extracted from the AQ-IL$^-$ and AQ-IL$^{.2-}$ simulations.
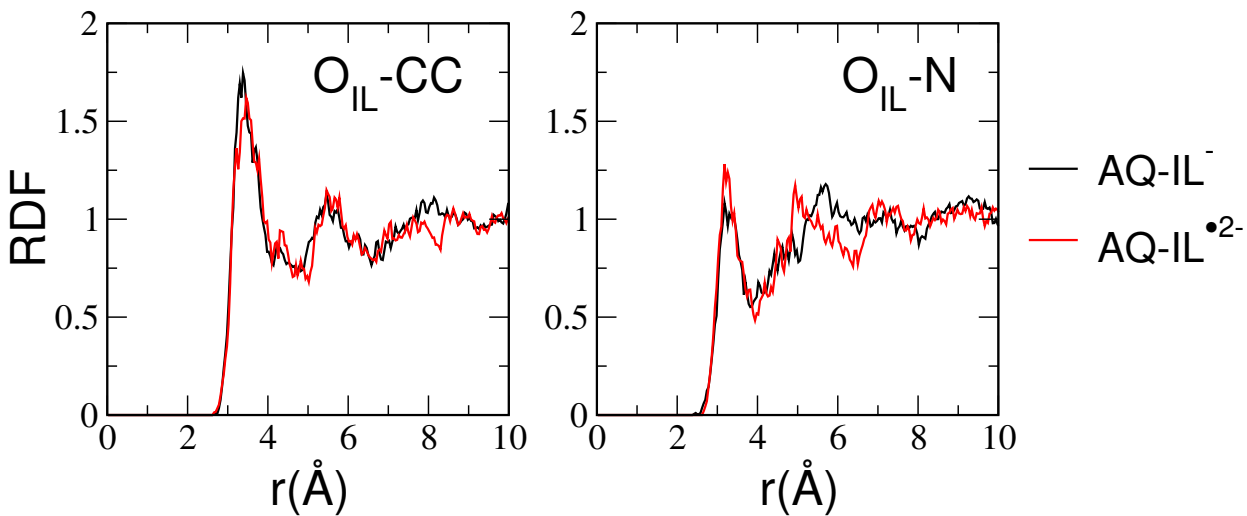

Figure S5. O_{IL}-CC (left) and O_{IL}-N radial distribution functions (RDFs). CC and N are the methyl carbon and nitrogen atoms of the acetonitrile, respectively. O_{IL} are the three oxygen atoms of the SO_3^- group belonging to the IL part.