Supplementary Information for

On the Mechanism of the Iodide-Triiodide Exchange Reaction in a Solid-State Ionic Liquid

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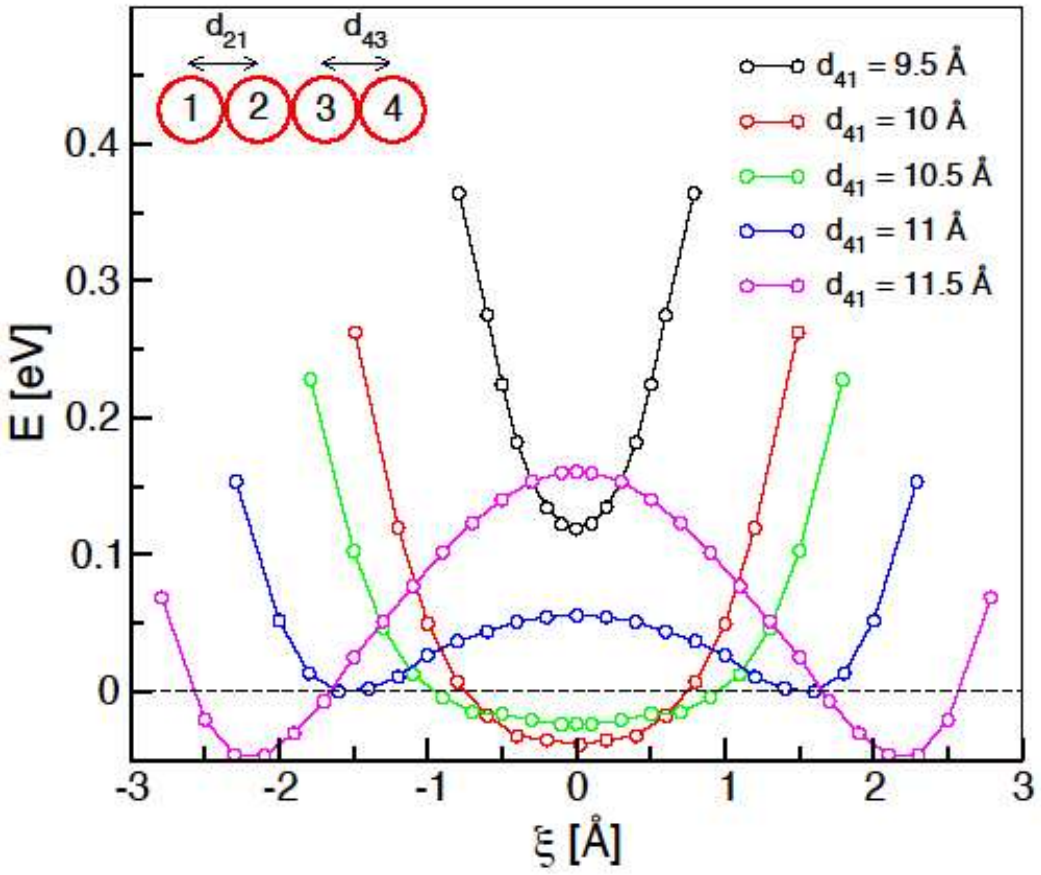

Fig. S1: Gas-phase study of the system potential energy as a function of ξ, for various d_{41} separations, via DFT single-point calculations. A collinear arrangement is adopted

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for ‘head-on’ approach of 1 and departure of 4. For d_{41} is less than, or up to, ~10.5 Å, a single energy minimum is evident for $\xi = 0$ (*i.e.*, $d_{43} = d_{21}$), associated with the formation of a symmetric I_4^{2-}. Once d_{41} exceeds ~10.5 Å, two minima develop, for $I^-\cdots I_3^-$ and $I_3^-\cdots I^-$ (the approach of I^- 1 and departure of I^- 4, respectively).

Files labelled as **configure_x.pdb** contain the configurations used as initial/final state in the five concatenated NEB calculations of Figure 2.

Files labelled as **Reorientation_x.pdb or Exchange_x.pdb** contain the full set of atomic coordinates for each of the five NEB windows of Figure 2.