Supplementary Information (SI) for Physical Chemistry Chemical Physics.

Theoretical Evaluation of Na_2MgCl_4 Double Chlorite as an Electrolyte for All-Solid-State Sodium Ion Batteries

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Supplementary Information

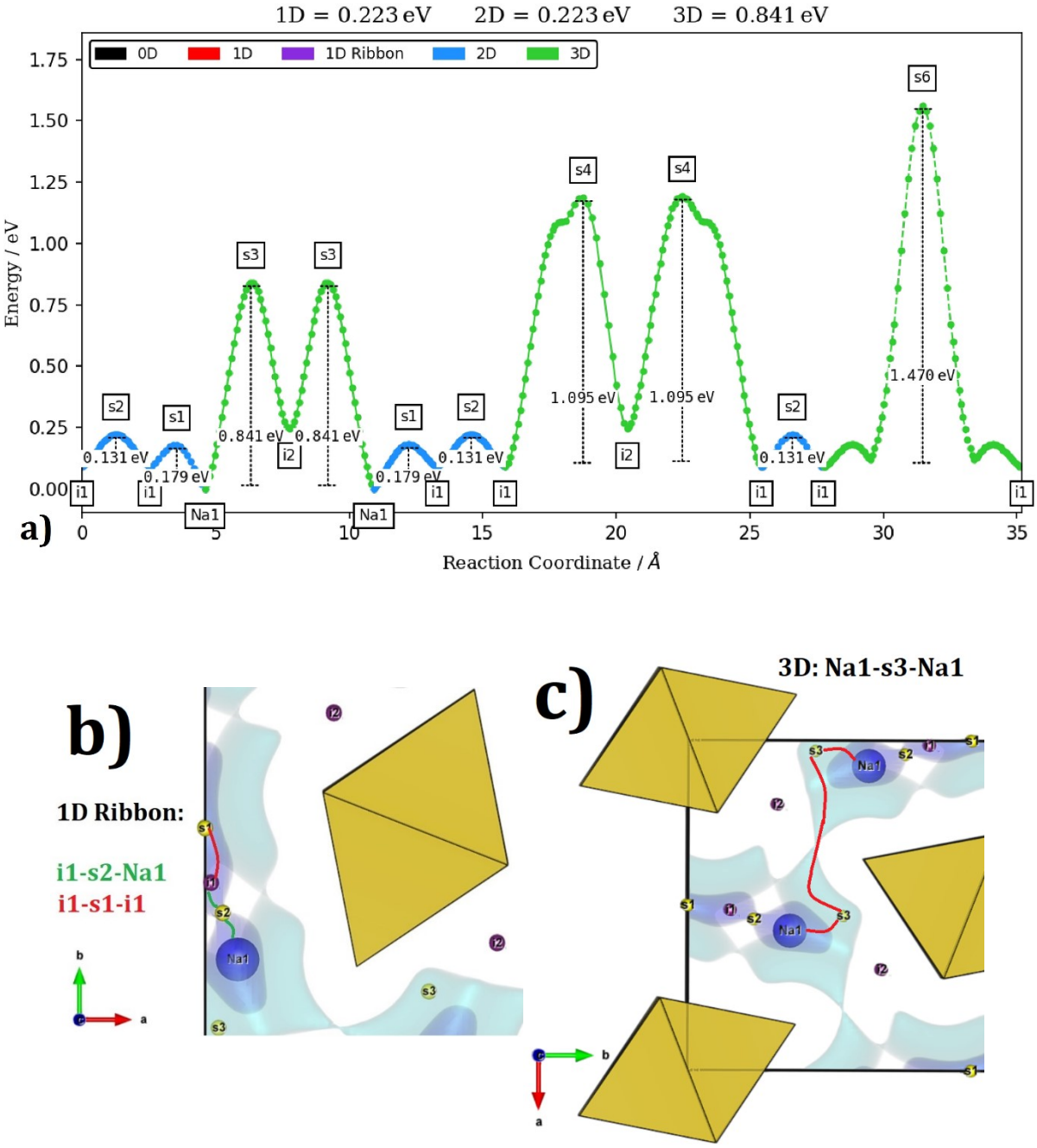

Fig. S1: **a)** Energy vs. reaction coordinate profile of Na_2MgCl_4, showing the 3D network of Na^+ migration pathways (blue isosurfaces) calculated by bond valence site energy. **b)** 1D ribbons and **c)** 3D migration pathways. The yellow polyhedral in panels **b)** and **c)** represent the [MgCl4] octahedral.

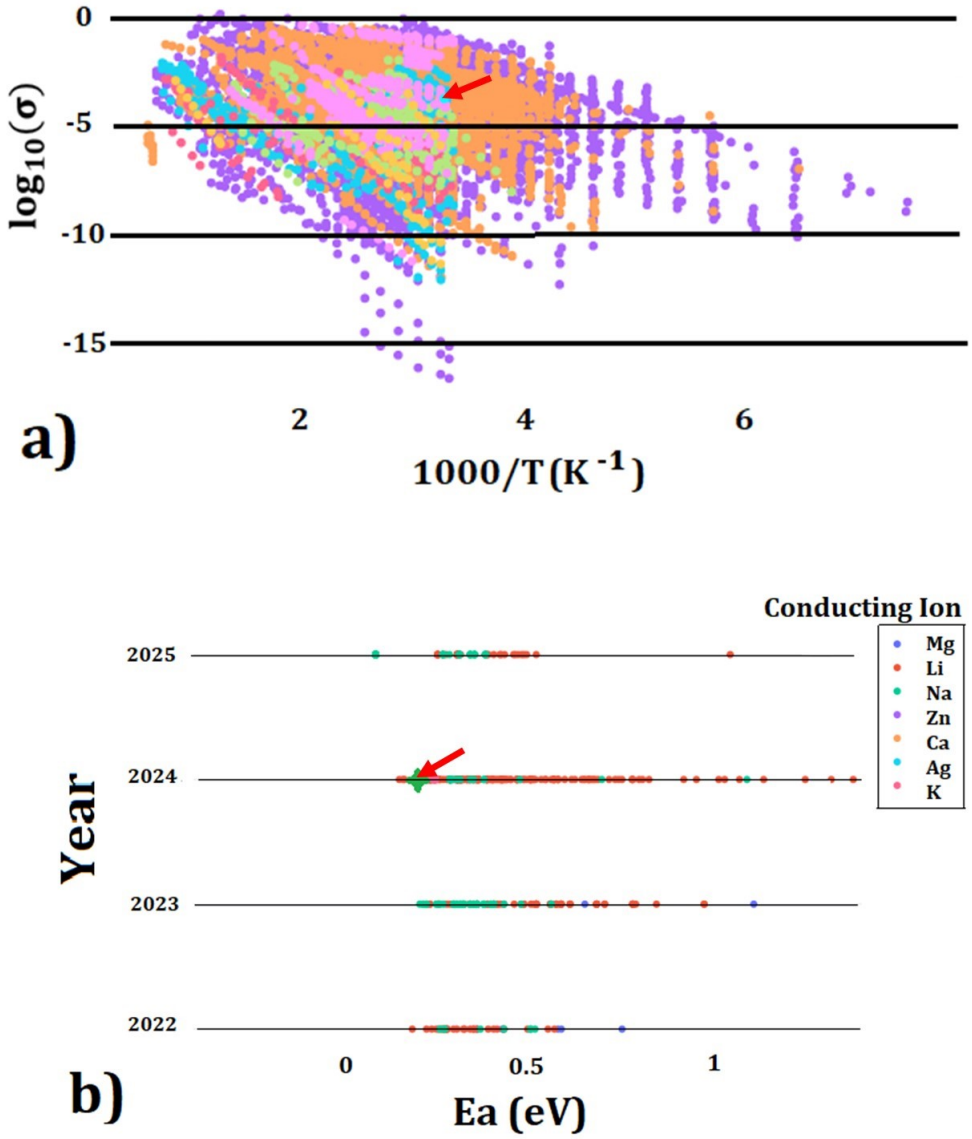

Fig. S2: Performance ranking of Na_2MgCl_4 based on **a)** room-temperature conductivity (σ) and **b)** theoretical activation energy (Ea), as reported in the Dynamic Database for Solid State Electrolyte (DDSE). The red arrow denotes the activation energy and room-temperature conductivity specific to Na_2MgCl_4.