Fast Mg^{2+} Diffusion in $Mo_3(PO_4)_3O$ for Mg Batteries –Supplementary Materials–

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S1 Computational Methods

All the DFT calculations were performed within the Vienna Ab initio Simulation Package (VASP). The Perdew–Burke–Ernzerhof (PBE)[1] form of the generalized gradient approximation (GGA)[2] was used for the exchange correlation energy, unless otherwise specified. Core electrons were incorporated using the projector augmented wave method[3], and valence electrons were expanded in the plane wave basis set. The energy cutoff of the plane waves was 520 eV for structure optimization and 400 eV for molecular dynamics. The Brillouin zone integration was performed with a *k*-space mesh of (3×3×1) for a (1×1×2) supercell. The AIMD simulations were run in a canonical ensemble with the Nosé–Hoover thermostat. The temperature fluctuation was controlled using a period of 40 time steps. The

time step was set to 1 fs for the Verlet integration. The diffusivities of both the MD and kMC trajectories were calculated using the diffusion analyzer module in the pymatgen package[4]. The nudged elastic band method (NEB) was used to find saddle points.[5, 6] Metastable sites along the migration path (A, B, C, D in Fig. 2) were well- relaxed and used as end points to segment the whole migration path into multiple NEB calculations. 5 images are used to interpolate each sub-path.

References

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