Supporting Information

Computational Screening of Oxide Perovskites as Insertion-Type Cathode Material

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Data Availability

NEB Images of MgNbO₃
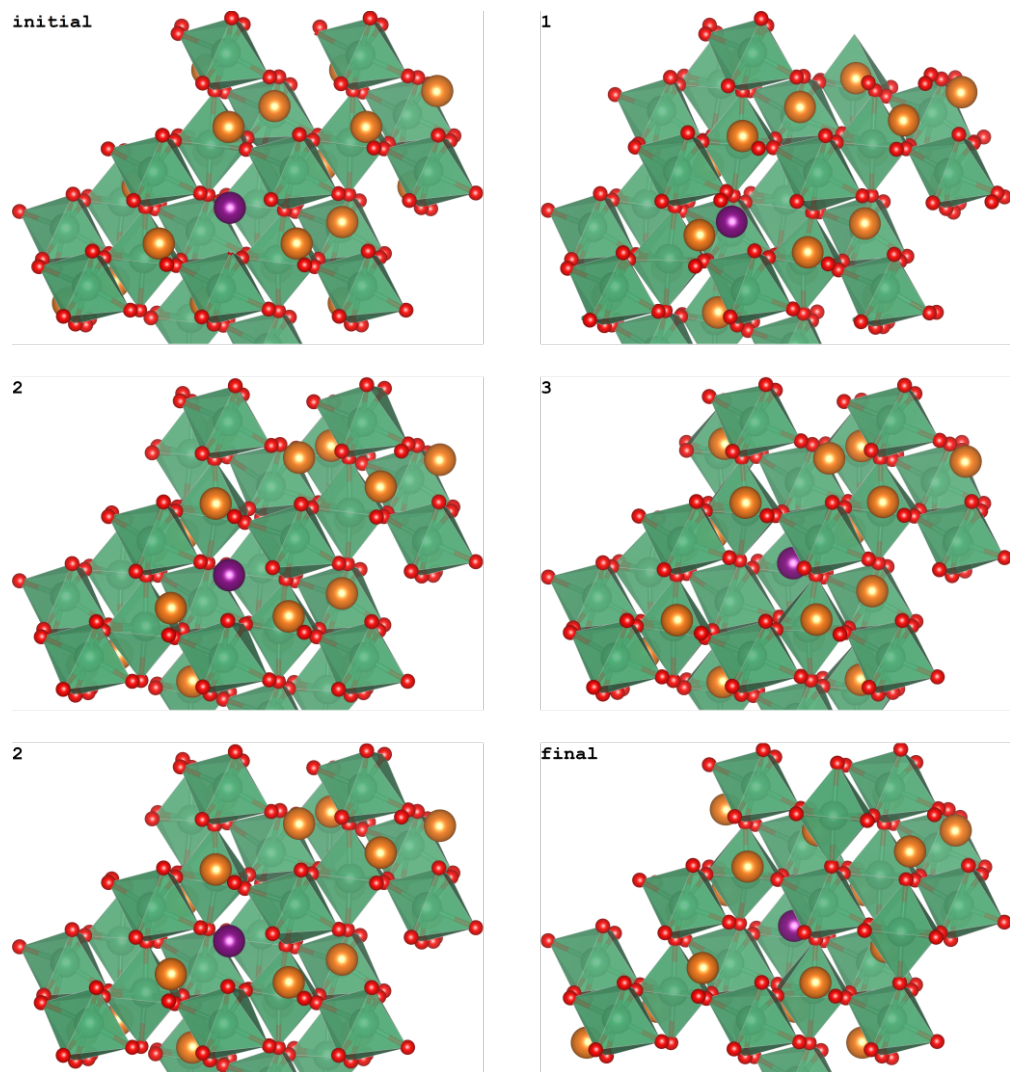

Figure 1: Visualisation of the diffusion path of MgNbO₃. All distinct images of the NEB calculation have again been geometry optimized in order to exclude any error of the NEB calculation. All structures retain the perovskite typical corner sharing octahedra.
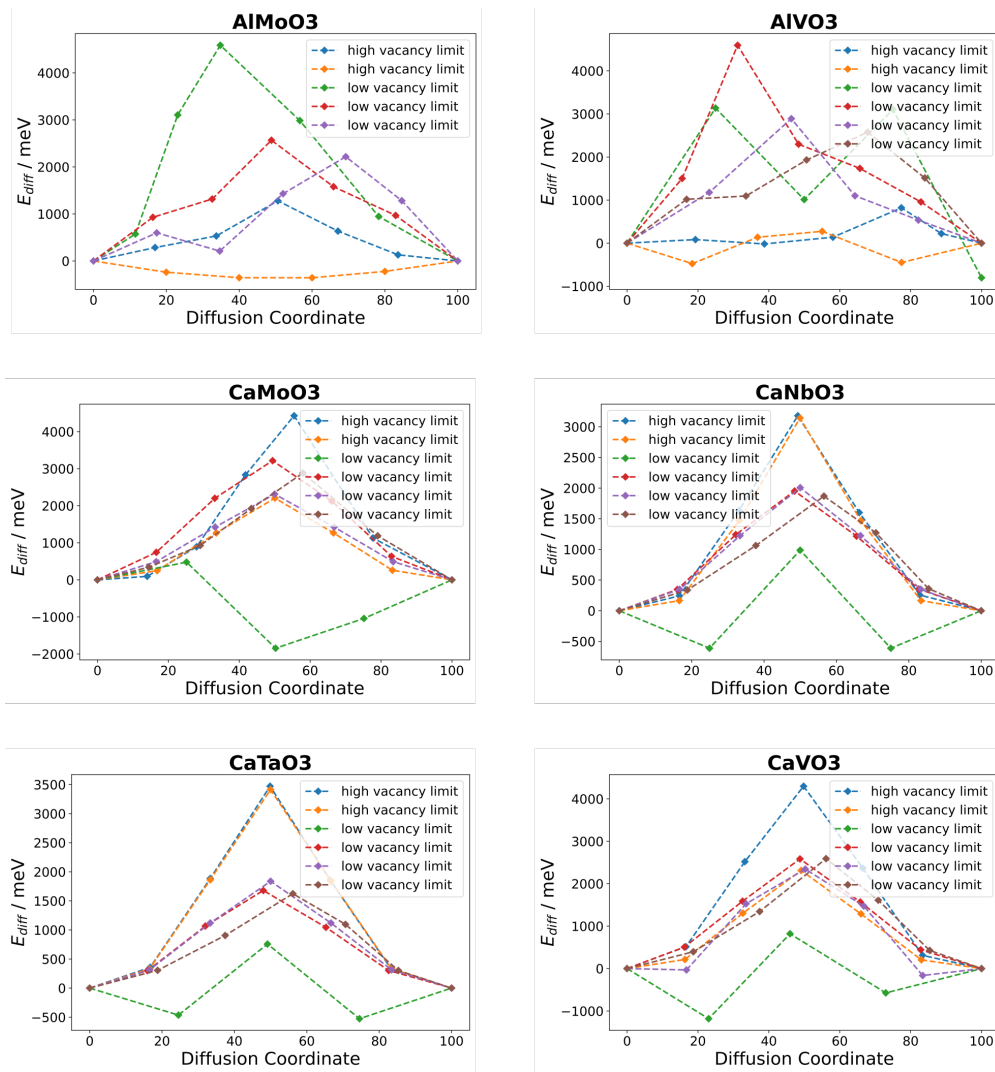
Diffusion barriers

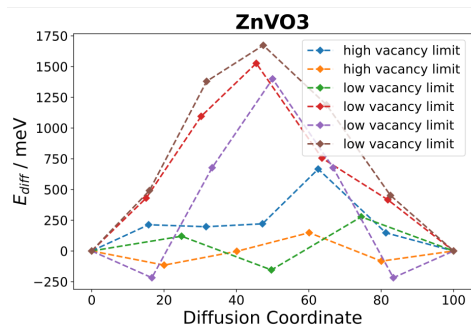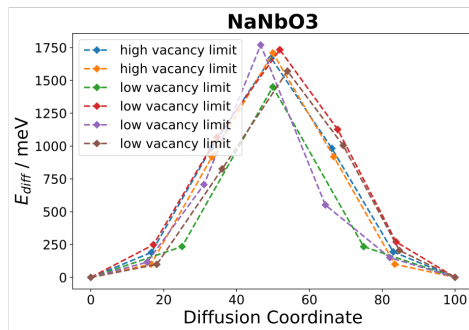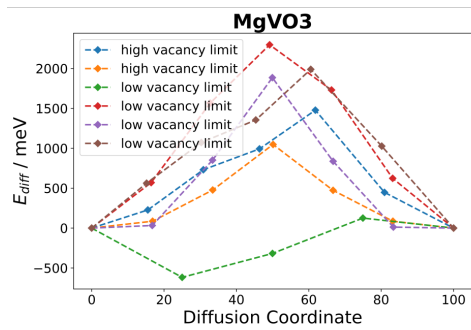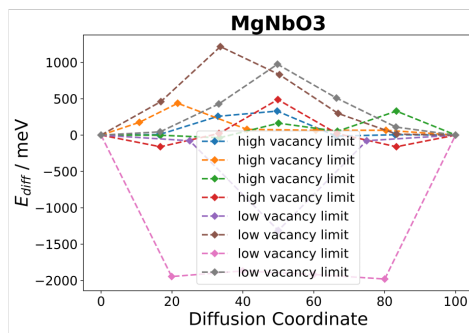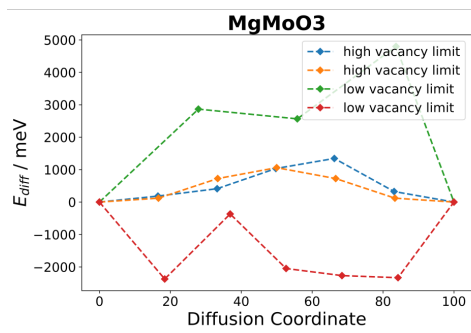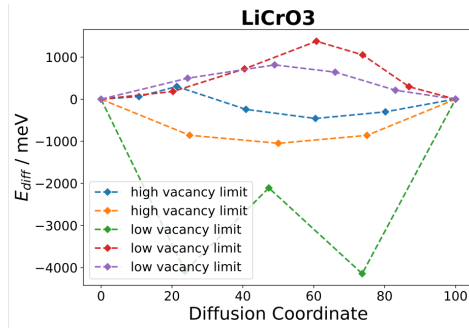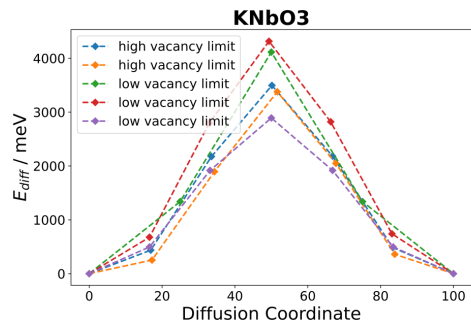Figure 2: Diffusion barriers of all compounds.

Figure 3: Diffusion barriers of all compounds - continued.