

# Supporting Information

## Computational Screening of Oxide Perovskites as Insertion-Type Cathode Material

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### Data Availability

All electronic structure calculations used in this work are made available under the Creative Commons Attribution license (CC BY 4.0) on the NOMAD repository (<https://nomad-lab.eu>) within the dataset “Johannes\_Doehn\_Oxide\_Perovskites”.

# NEB Images of $\text{MgNbO}_3$

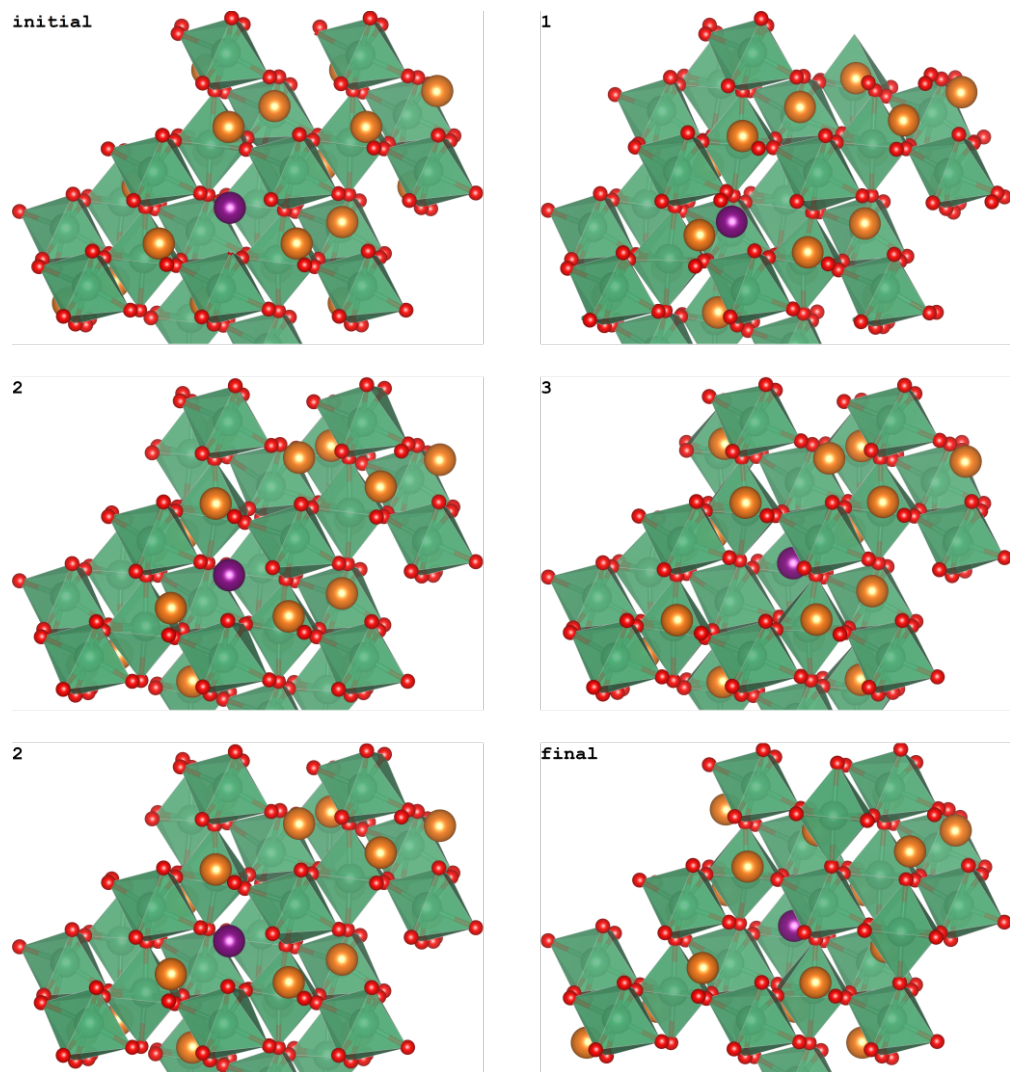


Figure 1: Visualisation of the diffusion path of  $\text{MgNbO}_3$ . All distinct images of the NEB calculation have again been geometry optimized in order to exclude any error of the NEB calculation. All structures retain the perovskite typical corner sharing octahedra.

# Diffusion barriers

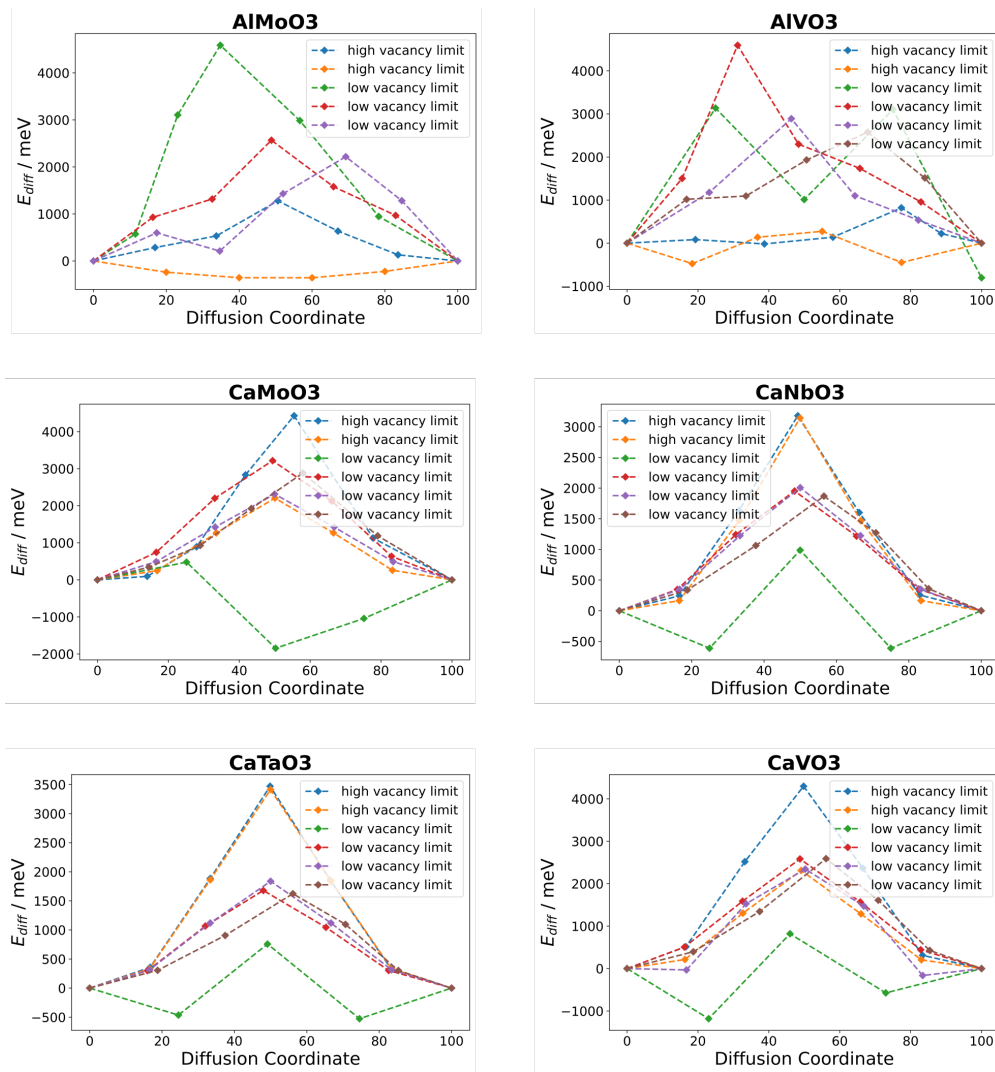


Figure 2: Diffusion barriers of all compounds.

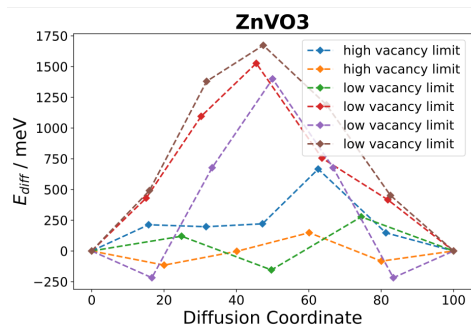
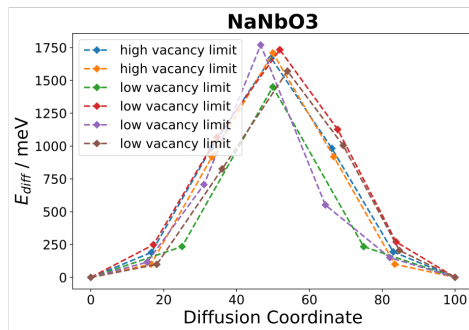
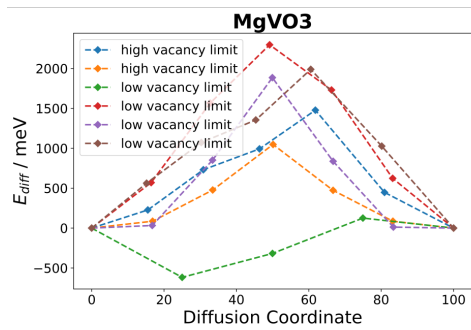
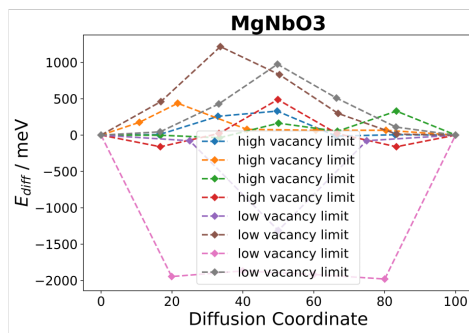
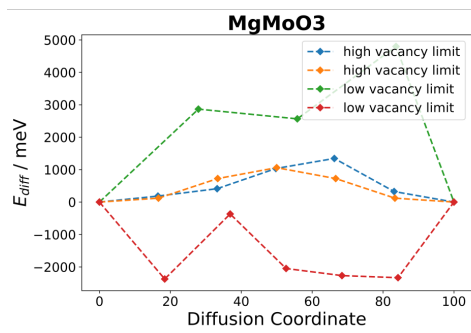
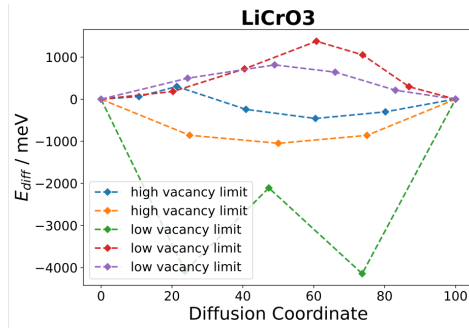
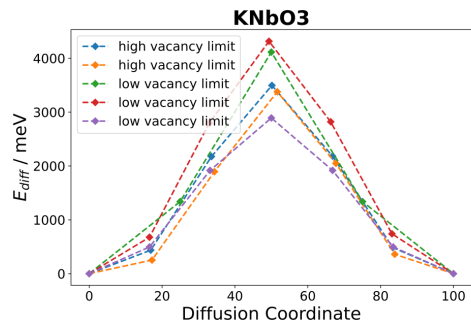


Figure 3: Diffusion barriers of all compounds - continued.