

Description of Additional Supplementary Files

Supplementary Data 1: List of CP2K Input Files

1. BASIS_SET: basis set file in the CP2K format
2. POTENTIAL: pseudopotential file in the CP2K format
3. NEB_FEPOR_Li.inp: nudged elastic band simulation file
4. FEPO4_Li_Initial_State.xyz: geometry file of the initial state in the XYZ format
5. FEPO4_Li_Final_State.xyz: geometry file of the final state in the XYZ format