

Title of the related article: Unraveling the Electronic Control of Hydride Diffusivity in Oxyhydrides from Model Studies on BaTiO₃-xHy

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Description of dataset:

This dataset contains input and output files of the DFT package Vienna Ab initio Simulation Package (VASP) used to generate the results of the related article.

Version of VASP used: vasp.5.4.4.18.

Input files are: INCAR, POSCAR and KPOINTS files. They contain the VASP setting parameters, the atomic positions in the supercells, and the k-points grid used, respectively.

Output files are OUTCAR files. They contain information about the calculated forces, energies, and atomic position.

The detailed content of these files can be understood with the VASP manual (https://www.vasp.at/wiki/index.php/The_VASP_Manual).

The files are sorted in folders and subfolders using the following keywords:

- 2x2x2_supercell, 3x3x3_supercell, and channel_supercell relate to the type of supercell used in the calculation.
- PBEsol, PBE+U, and HSE06 relate to the functional used in the calculation.
- -cell-optimization designates a structure optimization calculation.
- -elecBand designates an electronic band structure calculation.
- -dos designates an electronic density of state calculation.
- -NEB designates a nudged elastic band calculation.
 - 01, 02, 03 subfolders designate the initial state, transition state, and final state of the NEB calculation.
- -TS designates a calculation conducted at the transition state.
- -333kmesh designates a calculation using a 3x3x3 k-points mesh.