Skolkovo Institute of Science and Technology

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Computational Chemistry
Your project title

Final project report

Students :
Your name

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Supervisor
Name of your supervisor

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Contents

1 Introduction

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As shown in fig. 1.

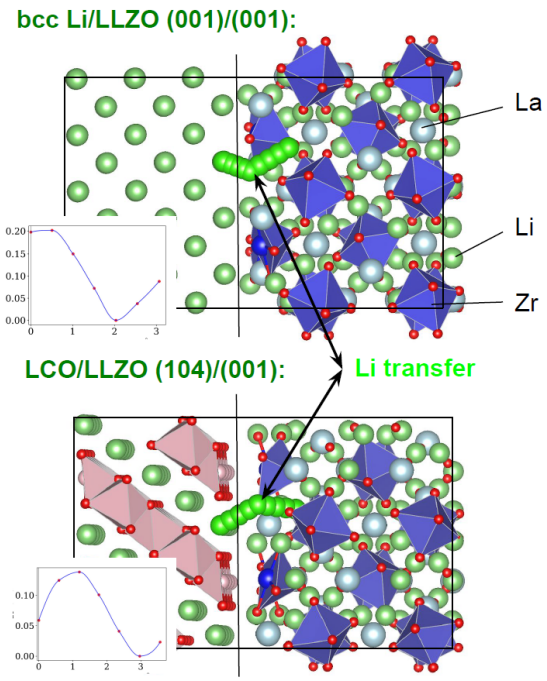

Figure 1. Interfaces in Li/LLZO and LCO/LLZO supercells.

2 Methods and parameters

2.1 First-principle calculations

To find energies of non-stoichiometric surfaces, we calculated surface energy as follows:

$$\gamma = \frac{1}{2A}\left[G_{\text{surface}} - G_{\text{bulk}} - \sum_{i}^{\text{species}} \Delta n_i \mu_i\right], \tag{1}$$

where A is the surface area in m^2, G_{surface} and G_{bulk} are the surface free energies of periodic surfaces and the reference bulk material, respectively; n_i and μ_i are the chemical potential and number of non-stoichiometric atoms of species i.

2.2 Calculation details

To find G_{surface} and G_{bulk} with used Vienna Ab initio Simulation (VASP) [1] package to perform density functional theory (DFT) calculations. All DFT calculations were performed within the generalized gradient approximation (GGA) in the Perdew–Burke–Ernzerhof (PBE) form [2, 3] for the exchange-correlation functional. The electron–ion interaction is described with the projector augmented wave (PAW) method [4]. For atoms of Li, La, Zr, and O, we considered 1, 11, 4, and 6 valence electrons, respectively. All the calculations were performed with cutoff energy $E_{\text{cut}} = 300$ eV. The smearing method was chosen as Gaussian for the reason of LLZO being a wide gap insulator. K-point spacing was chosen as 0.7 Å. This parameter is sufficiently accurate for large cells and allowed us to reduce the computational time compared with more precise k-mesh. The conditions of convergence were 0.05 eV/Å for forces and one-thousandth 10^{-3} eV/atom.

3 Results and discussion

3.1 Thermodynamic stability

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Example of citations [4, 2, 3].

3.2 PDOS

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4 Conclusions

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