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Theoretical Study of the Catalytic Properties of $BaTiO_3$ as Anode for Solid Oxide Fuel Cell

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【Introduction】

The most efficient solid oxide fuel cell (SOFC) catalyst (Nickel – Yttria Stabilized Zirconia) up to date presents some disadvantages that lower its activity for the electrochemical oxidation of fuels such as deactivation due to H_2S poisoning [1], carbon deposition [2], because YSZ is pure ionic conductor the oxidation step is limited to the three-phase-boundary, and at the current operating temperatures Ni tends to agglomerate [3]. For the aforementioned reasons we are studying the possibility of a new Ba based material as anode for SOFC.

【Method】

For all the calculations in this study we employed VASP v5.3.3, PBE-GGA was employed using the PAW pseudopotentials and a plane wave energy cut-off of 400 eV was set for all calculations. The $BaTiO_3$(001) surface was modeled with four altering TiO_2 and BaO in a 2x2 supercell, the vacuum slab was set to 15 Å. The optimization was performed employing 4x4x1 k-point mesh for both terminated slabs, BaO-terminated (BaO^T) and TiO_2-terminated (TiO_2^T) where the atoms of the two bottom layers were kept frozen. For the interaction of the adsorbate with the adsorbent a set of 4x4x1 k-point mesh was used.

【Results and Discussion】

We found that H adsorption is more stable on TiO_2^T than on BaO^T. Moreover, when two H atoms interact with the surface of either BaO^T or TiO_2^T they will form H_2O and an oxygen vacancy (Figs. 1a and 1b). Also, for the case of H_2 on BaO^T we observed the formation of H_2O and an oxygen vacancy (Fig. 1c). When H_2 interacts with TiO_2^T we observed the dissociation of the molecule to form two OH^- in the surface (Fig. 1d). In addition, we found that CH_4 is adsorbed more stably on TiO_2^T, nevertheless the value is minor. We also studied the interaction of H_2S with both surface noticing how one of the H detach from H_2S to bond with the O from both surfaces to form OH^- (Fig. 1e). For the case of TiO_2^T we observed that the remaining HS^- will bond with the surface Ti (Fig. 1f).

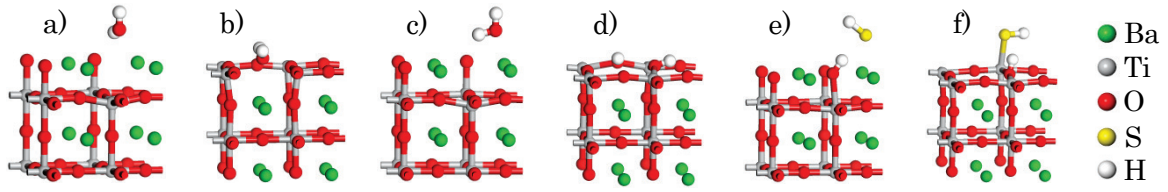

Fig. 1 Optimized structures of the interaction of a) two H with BaO^T, b) two H with TiO_2^T, c) H_2 with BaO^T, d) H_2 with TiO_2^T, e) H_2S with BaO^T, f) H_2S with TiO_2^T.

【References】

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