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Behavior of the native defects and hydrogen impurities in SnO_2

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Abstract – Native defects (V_O, V_{Sn}, Sn_i, O_i, O_{Sn}, Sn_O) and the hydrogen impurity (H_i, H_O, H_{Sn}) in the rutile structure of SnO_2 are investigated, owing to the possibility of the defects and impurities act as a donor depending on the occupied site. It is provided a systematic analysis of the several systems studied also varying the charge state of the defects and of the hydrogen impurity. Results have been obtained by performing ab initio electronic structure calculations based on the Vienna Ab-Initio Simulation Package and the projector augmented wave (VASP-PAW) methods within the density functional theory and the local density approximation.

Tin dioxide (SnO_2) is a transparent conducting oxide (TCO) and has been highly utilized in optoelectronic devices, gas sensors, flat panel displays, etc., due to its high conductivity and transmission. It has a direct band gap of 3.6 eV and when not intentionally doped shows a n-type semiconductor character, likely due to native defects, such as oxygen vacancies and interstitial or substitutional tin. Another possibility for the sample n-type character is related to hydrogen defects, althougt there is no direct experimental evidence of the hydrogen hole and a controversial theoretical point of view exists [1,2,3]. Here, we present a theoretical investigation on the physical properties of native defects (V_O, V_{Sn}, Sn_i, O_i, O_{Sn},Sn_O) and hydrogen impurities (H_i, H_O, H_{Sn}) in the rutile structure of SnO_2 to investigate their donor character. The calculations are based on the density functional theory in local density approximation (LDA) with generalized gradient corrections (DFT-GGA) according to Perdew-Burke-Ernzerhof. The electron-ion interaction is described by pseudopotentials generated with the Projector-Augmented-Wave scheme, as implemented in the Vienna Ab-initio Simulation Package (VASP-PAW). The Sn 4d, 5s, and 5p and O 2s and 2p electrons were treated as valence band states. On-site Coulomb correlations interaction was including in Sn 4d orbital. The equilibrium structure was obtained by relaxing the system with respect to the lattice parameters *a*, *c/a*, and *u*. The obtained values are a = 4.730 A, c/a =0.669 , and u = 0.306, in good agreement with the experimental data.
The electronic structure calculations of the native defects and hydrogen impurities were simulated by using the theoretical equilibrium lattice parameters of the rutile structure in a 72-atom supercell with a 490 eV cutoff energy in the plane-wave expansions and a 2x2x2 mesh of Monkhorst-Pack k-points for integration in the Brillouin Zone. We have investigated the atomic structures, symmetries, and formation and transition energies of the defects and impurities, to verify if some of them can act as donor centers, and were compare with available results.

References

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