Structural and electronic properties of europium-doped SnO_2: first principle insights

Felipe Mondaca [1*], Francisco Calderón [2], Sergio Conejeros [3] and Arturo Martínez [4]

[1]Facultad de Ingeniería, Arquitectura y Diseño, Universidad San Sebastián, Lago Panguipulli 1390, Puerto Montt, Chile.
[2]Departamento de Física, Universidad Católica del Norte, Avda. Angamos, 0610, Antofagasta, Chile.
[3]Departamento de Química, Universidad Católica del Norte, Avda. Angamos, 0610, Antofagasta, Chile
[4]Centro de Investigación y de Estudios Avanzados del IPN Unidad Saltillo, Av. Industria Metalúrgica 1062, Parque Industrial Ramos Arizpe, 25900, Coahuila, México.

*felipe.mondaca@uss.cl

Abstract

The CRYSTAL17 code [1] was used to apply the density functional theory (DFT) to rutile tetragonal tin oxide (SnO_2) with space group P_{42}/mnm. First, the crystalline structure of SnO_2 was modeled in a unit cell, which contains 2 atoms of tin and 4 atoms of oxygen. We employed different bases using the PBE functional to have a greater agreement with the lattice constant experimental. Second, in order to investigate the impacts of the Eu^{3+} impurity, the SnO_2 structure, with an oxygen vacancy (V_O) and two europium (Eu) atoms, was meticulously modeled in a 3×3×2 supercell ($Eu_2Sn_{34}O_{71}$). The total energies of multiple $Eu_2Sn_{34}O_{71}$ supercell configurations were calculated and compared. It was discovered that when two Eu atoms are bonded through an oxygen atom and the V_O is bonded to an Eu atom, the total energy is at its lowest. To account for the six unpaired *f* electrons in the Eu^{3+} cations, all Eu-doped supercell simulations were spin-polarized. The electronic properties such as the band structure, density of state (DOS), bandgap, and effective mass were predicted using HSE06 functional. The band structure and DOS predicts that SnO_2 and $Eu_2Sn_{34}O_{71}$ supercells exhibit insulator character. Furthermore, the $Eu_2Sn_{34}O_{71}$ supercell permits intraband *f-f* transitions that are otherwise prohibited in atomic Eu. This result is consistent with photoluminescence (PL) found for Eu-doped SnO_2 (ETO) films and nanoparticles in the visible red range. The characteristics of the ETO compound suggest that it could be a suitable phosphor material for reducing thermalization losses in solar cells [2].

Acknowledgements:
We would like to thank "Núcleo de Investigación No.7 UCN-VRIDT 076/2020, Núcleo de modelación y simulación científica (NMSC)" for the scientific support. F.A.C acknowledges support from CONACYT PAI 79170075. S.C. was supported by FONDECYT (Chile) through project 11171063.

References

[1] See, https://www.crystal.unito.it
[2] Y. Zhang, X. Jia, S. Liu, B. Zhang, K. Lin, J. Zhang, and G. Conibeer, Sol. Energy Mater. Sol. Cells. 225, 111073 (2021)