Efect of oxygen vacancies in bismut oxide Energy-Loss Near-Edge Structure spectra by ab initio simulations

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Idioma Indefinido

Descrição:

Proyecto asignado a través de la Red Española de Supercomputación [2].

The present work summarizes the results of combining experimental Electron Energy Loss Spectroscopy measurements and Density Funtion Theory (DFT) simulations to detect and quantify oxygen vacancies in bismut oxide nanowires. The combination of experimental results and ab initio calculations give the possibility of understanding the optoelectronic properties of the sample and, since, one can control the percentage and the position of oxygen vacancies, it allows to analyze their effect. The theoretical calculations of the electronic structure were carried out using the linearized augmented plane wave (LAPW) method based on DFT, implemented on WIEN2k ab initio simulation package.

Journals and conferences:

- Assessing Oxygen Vacancies in Bismuth Oxide through EELS Measurements and DFT Simulations [3].
  Pau Torruella, Catalina Coll, Gemma Martín, Lluís López-Conesa, María Vila, Carlos Díaz-Guerra, María Varela, María Luisa Ruiz-González, Javier Piqueras, Francesca Peiró, and Sònia Estradé.
  The Journal of Physical Chemistry C [4] 2017 121 (44), 24809-24815.
  DOI: 10.1021/acs.jpcc.7b06310 [5].

Ligações

[1] http://www.ub.edu/ [2] https://www.res.es/ [3] http://www.cenits.es/enlaces/publicaciones/assessing-oxygen-vacancies-bismuth-oxide-through-eels-measurements-and-dft [4] http://pubs.acs.org/journal/jpccck [5] http://dx.doi.org/10.1021/acs.jpcc.7b06310