
Assessing Oxygen Vacancies in Bismuth Oxide through EELS Measurements and DFT Simulations

Pioneering electron energy loss spectroscopy (EELS) measurements of α -Bi₂O₃ are performed on three samples obtained through different synthesis methods. Experimental low-loss and core-loss EELS spectra are acquired. By combining them with detailed structural characterization and Density Functional Theory (DFT) simulations, we are able to detect and evaluate the presence of oxygen vacancies in the samples. This type of information has not been accessed previously from EELS data in bismuth oxide, because high-resolution EELS spectra or how vacancies reflect in Bi₂O₃ spectra were unreported. This novel measurement is further validated through comparison with photoluminescence data. Therefore, the technique has the ability to probe oxygen vacancies in Bi₂O₃ at an unprecedented resolution, which might allow solving material science and technological issues related to this material.

Fuente de la publicación:

- Assessing Oxygen Vacancies in Bismuth Oxide through EELS Measurements and DFT Simulations. 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](#) [1] 2017 121 (44), 24809-24815. DOI: [10.1021/acs.jpcc.7b06310](https://doi.org/10.1021/acs.jpcc.7b06310) [2].

Proyectos relacionado:

- [Effect of oxygen vacancies in bismuth oxide Energy-Loss Near-Edge Structure spectra by ab initio simulations](#) [3].

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[1] <http://pubs.acs.org/journal/jpccck> [2] <http://dx.doi.org/10.1021/acs.jpcc.7b06310> [3] <http://www.cenits.es/proyectos/efect-oxygen-vacancies-bismuth-oxide-energy-loss-near-edge-structure-spectra-ab-initio>