
Ab-initio based data mining techniques for studying the emergent phenomena in $\text{La}_{1-x}\text{Sr}_x\text{MnO}_3/\text{BaTiO}_3$ heterojunctions

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Idioma Indefinido

Descrição:

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

Oxide heterojunctions (OH) constitute a material framework where interfaces often exhibit new phenomena unrelated to its constituents bulk properties. Involved mechanisms arise from the complex interrelation between lattice, charge, orbital and spin where no experimental technique can unravel the whole complexity. However, the increasingly large information density (called datacubes) acquired in scanning transmission electron microscopy and electron energy-loss spectroscopy contains more and more details of the subtle mechanisms involved. We tackle the problem using “big data” techniques applied to ab-initio simulations which can help rationalizing those datacubes into a reduced set of configurations in the real (energy) space towards a realistic description of structural distortions (oxidation states) at the interface of OH.

Web:

URL de

origem: <https://web.computaex.es/pt-pt/proyectos/ab-initio-based-data-mining-techniques-studying-emergent-phenomena-la1-xsrxmno3batio3>

Ligações

[1] <https://www.ucm.es/> [2] <https://www.res.es/>