Ab-initio simulation of the electronic and magnetic properties in iridate-based oxide heterostructures

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Description:

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

Oxide heterostructure (OH) with spin-orbit-coupling like SrIrO3/SrTiO3 have the potential to be designed as topological insulators, either band or Mott types. This roots on the properties exhibited by the iridates family of Ruddlesen-Proper series since the members with n=1,2,∞ are antiferromagnetic (AFM) Mott insulator, AFM band insulator and paramagnetic semimetal phases respectively. There is a number of works relating the RPS properties and thin film configurations of strain and oxygen vacancies which could provide an atomic engineering path towards topological phases and transitions, however the topic is still at its infancy. This project aims to tackle this issue using simulation techniques efficient of providing an experimentally realistic scenario of the quantum mechanisms such as the octahedral distortion and bandwidth in OH.

Links

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