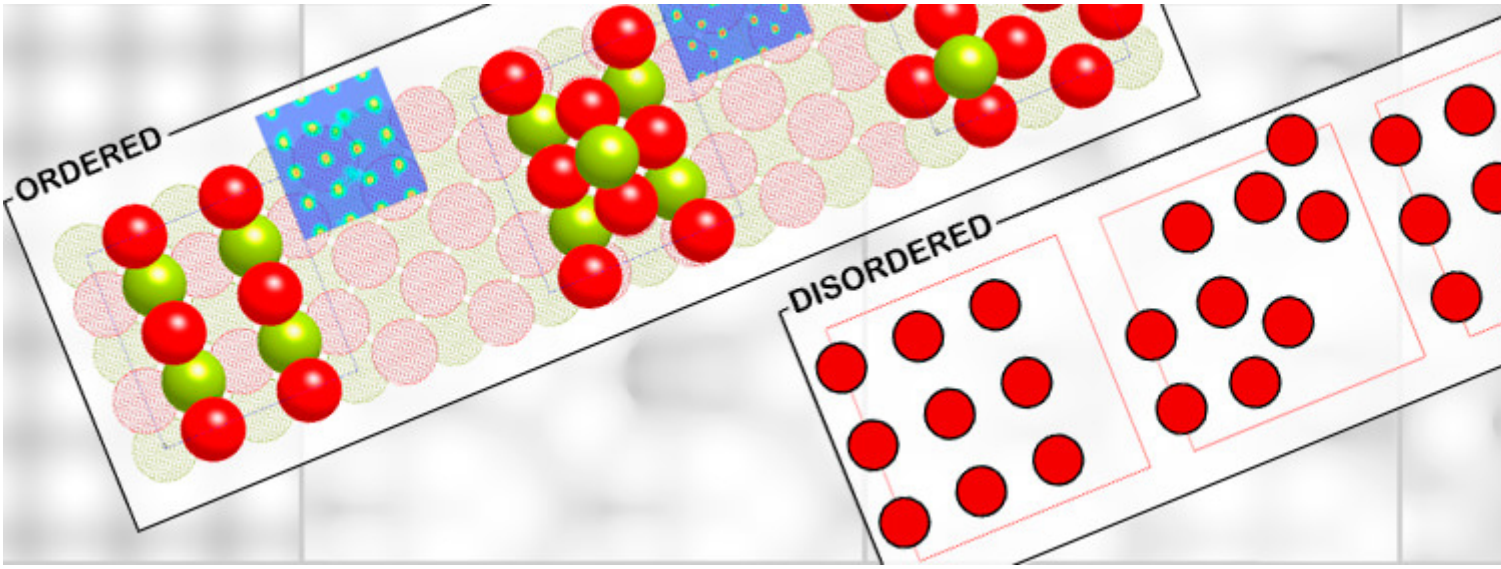
Researchers at ICIQ present a study in Nature Materials that demonstrates that surfaces might be disordered



(via ICIQ)

- The group of Prof. Núria López is a user of the MareNostrum supercomputer, which has contributed to the project more than 50,000 simulations.
- Drs. Marçal Capdevila-Cortada and Núria López have published a work in Nature Materials that describes the keys for the existence of intrinsic disordered structure on surfaces that can affect all their properties.
- The discovery can help improving the physical and chemical properties of oxides or other materials that can be applied in fuel cells and the catalysts already present in cars to abate pollutants, thus improving the air quality in cities.

Materials, particularly oxides, present surfaces where the positions of the atoms are typically ordered. The detailed knowledge of atom distributions allows the prediction of their properties and even tailoring them. However, for some of these materials the reality might depart significantly.

The group of Prof. Núria López, through massive computer simulations (more than 50,000) performed at the MareNostrum computer in the Barcelona Supercomputing Center, have shown that some surfaces present an intrinsic disorder that renders the prediction of their properties much more complex than initially thought. In this case, the use of simulations becomes essential, as they allow introducing all the complexity of these materials. The new findings complement the main role of disorder (entropy) in other areas of chemistry, physics, information technologies, and biology. The area is blooming, yet somehow entropy is a naturally difficult concept, as our brains are better suited to recognize patterns and symmetries.

The work published by the ICIQ researchers describes accurately why and how the surface atomic reorganization for polar surfaces takes place. Based on the configurational entropy schemes (that is, how

many possible configurations can appear for a given number of particles in a larger number of boxes), they classified different structure terminations by considering which are the most stable. Moreover, they have shown that at operation temperatures these surfaces are dynamic and thus the reordering is possible (Nature Materials DOI:10.1038/NMAT4804). The new surface structures present local structures that depart from the initial ones and can affect the mechanic, catalytic, and sensing properties of these materials. These physical and chemical properties are at the core of energy use improvement, and will allow to devise greener and more sustainable chemical processes that would pave the way for a circular economy.

Entropic contributions enhance polarity compensation for CeO_2(100) surfaces
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Nota en català
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