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Challenges in the modelling of oxides

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Oxides are active materials for multiple applications including catalysis and particularly for energy purposes. However, many properties are still not fully understood and fundamental questions regarding the structure are far from being known. In the present talk, I will give a description of key structural issues that might affect the properties of these materials.

Oxides constitute a class of active catalytic materials in chemical transformations some of them aimed at providing new energy vectors. Even the most fundamental questions regarding the nature, stoichiometry and structure of the surface of some oxide are intriguing. For ceria, a material widely employed as catalytic support, we have found that the termination of open, polar surfaces will be completely controlled by configurational entropy. This observation opens a wide new concept in the way we understand the properties of this class of materials.

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