Nanostructured materials | Jožef Stefan Institute Ljubljana, Slovenia

SEMINAR

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On the Surfaces of Complex Oxides

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Perovskite-type rare-earth metal oxides are being considered for use as air electrode materials in electrochemical devices operating at intermediate to high temperatures. Understanding the surface chemistry of these materials is crucial for determining the kinetics of oxygen reduction and exchange reactions. Among various perovskite-type complex oxides, certain members of the Ruddlesden–Popper series, such as La_2NiO_4, have shown significant activity for surface oxygen interactions. However, a challenge remains in identifying the structure and composition of active surfaces, as well as their influence on surface exchange mechanisms. In this presentation, changes in the electronic structure and energetics of oxygen interactions on La_2NiO_4 surfaces will be touched upon using Density Functional Theory (DFT) calculations. Recent experimental evidence suggests LaO termination, rather than NiO_2 termination, on the surfaces of rare-earth perovskite oxides after heat treatment in oxidizing environments, as they become transition metal-free. Computational findings support the idea that LaO-terminated surfaces can form surface superoxo species. Detailed charge transfer analyses indicate that such surfaces can be catalytically active due to enhanced electronic configurations on neighboring La sites interacting with surface species. Additionally, positively charged oxygen vacancies relative to the crystal lattice can serve as active sites, catalyzing O–O bond cleavage.

Kindly invited.