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Abstract

The Influence of Non-Stoichiometry on the Order and Dynamics of Oxides Studied by Inelastic Neutron Scattering †

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Oxygen ionic conductors are materials of fundamental interest for the development of ambient temperature working devices for energy conversion, such as solid oxide fuel cells (SOFC).

Inelastic and neutron scattering experiments, coupled with ab-initio molecular dynamics simulations (AIMD), give the unique chance to unveil the presence of specific low-energy modes favoring diffusion events and so explaining the unusual high mobility down to moderate temperatures.

Experiments and AIMD on Nd_2NiO_4 systems [1,2] allowed to depict the on-site motion of the diffusive species and understand the impact of oxygen over-stoichiometry on the lattice dynamics of the Nd_2NiO_4 framework. A recent analysis on a single crystal allowed us to go beyond and verify that this partially disordered non-stoichiometric system show both correlated and uncorrelated dynamics, quite surprising for a crystalline compound [3].

References

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