

# High-entropy oxides for energy-related applications

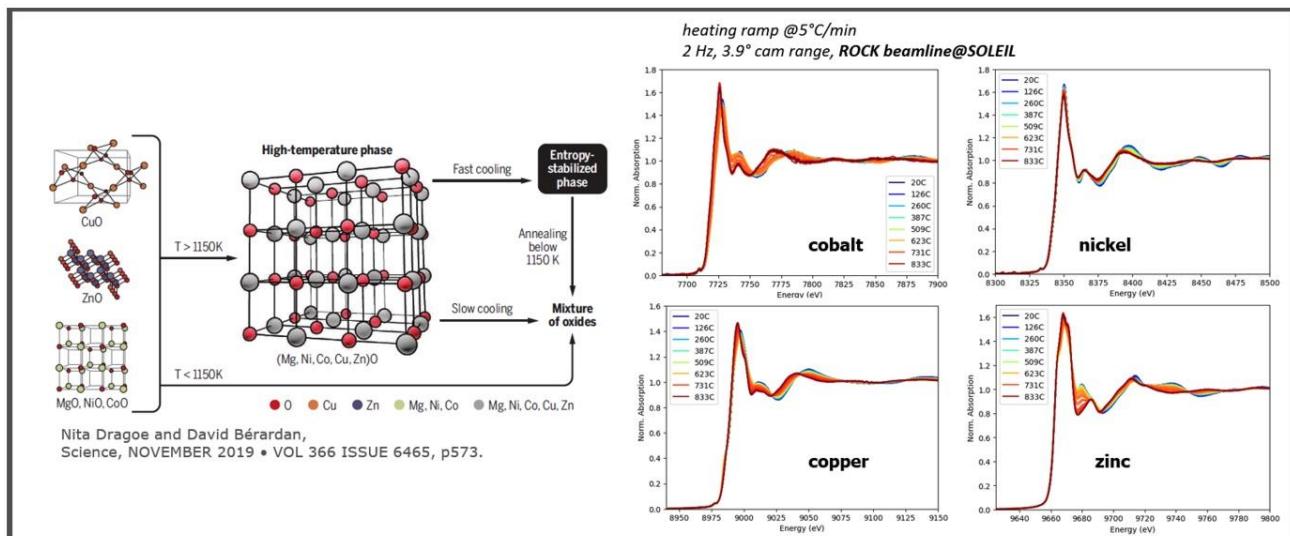
**Participants** : Isabelle Maurin, Denis Testemale, Christophe Lepoittevin

**Former students** : Jade Chongsathapornpong (MIT, Massachusetts), Jean-Baptiste Boucquiaux (IUT d'Orsay, Université Paris-Saclay)

Since their discovery (Rost *et al.*, *Nature* 2015), high entropy oxides (HEO) have become a promising playground to develop new functional materials. HEOs are generally produced by mixing several binary oxides, five or more, in near equimolar amounts. When heated at a temperature above which the configurational entropy dominates the Gibbs free energy term, a solid solution can be formed even from immiscible oxides. This *entropy concept* provides a versatile approach to design materials with properties that are often unique because they are driven by synergistic effects between the combined elements as recently shown in electrocatalysis for the oxygen evolution reaction (Baek *et al.*, *Nat. Commun.* 2023).

We are currently studying several HEO structure-types with different objectives:

- understanding the temperature path toward the multi-cationic oxide using advanced and time-resolved x-ray techniques at large facilities (ESRF, SOLEIL) to quantify the role of the mixing entropy through the identification of intermediate phases and to monitor the thermal stability of the mixed oxides
- correlating the structural and chemical disorder with functional properties (optical, magnetic, etc.)
- exploring new compositions as a route to sustainability and circularity of strategic materials



Schematic and experimental reaction path toward the entropy-stabilized  $(\text{Mg}_{0.2}\text{Co}_{0.2}\text{Ni}_{0.2}\text{Cu}_{0.2}\text{Zn}_{0.2})\text{O}$  compound from *in situ* X-ray absorption spectroscopy.

## Collaborations :

Nita Dragoe and David Bérardan (ICMMO, Université Paris-Saclay, Orsay) / Sandrine Tusseau-Nénez and Walid Mnasri (PMC, Ecole Polytechnique, Palaiseau) / Mauro Rovezzi (The FAME and FAME-UHD beamlines, ESRF, Grenoble) / Alain Ibanez (OPTIMA research team, Néel) / Jochen Fick (NOF research team, Néel) and Corinne Félix (POM technological pole, Néel)

## References :

*Synthesis of  $(\text{MgCoNiCuZn})\text{O}$  entropy-stabilized oxides using solution-based routes: influence of composition on phase stability and functional properties*, W. Mnasri, D. Bérardan, S. Tusseau-Nénez, T. Gacoin, I. Maurin and N. Dragoe, *J. Mater. Chem. C* 2021, 9, 15121-15131, [doi.org/10.1039/D1TC03287A](https://doi.org/10.1039/D1TC03287A)