DIPARTIMENTO DI SCIENZE CHIMICHE

UNIVERSITÀ DEGLI STUDI DI PADOVA

15 maggio ore 10.30
Aula N, Dipartimento di Scienze Chimiche

Seminario

Extending the materials engineering space for energy applications by multicomponent equiatomic oxides

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Multicomponent equiatomic oxides, often called high entropy oxides (HEOs), represent a new class of materials that exhibit outstanding unique and tunable properties, making them promising for future applications for efficient energy conversion and storage. HEOs are complex single-phase oxides consisting of five or more cations in approximately equal amounts. Thereby, the metal cations arrange randomly on the cation lattice of the crystal structure, resulting in high configurational entropy. Even compositions that have a positive enthalpy of formation can be stabilized at a certain temperature when the entropy term of the Gibbs energy becomes larger than the enthalpy term, so-called entropy stabilization, extending the materials engineering space. Since the first publication in 2015 by Rost *et al*.,[1] many compositions and crystal structures have been synthesized with this approach, leading to novel materials with improved or unprecedent material properties most recently in the case of high-temperature, electrocatalyst-, battery and piezoelectric materials.
Due to the potential high configurational entropy and the resulting high-temperature stability, HEOs are promising materials for future thermal barrier coatings (TBCs) applied on the metallic alloy substrates in gas turbines. Using multiple different cations, their properties such as thermal expansion coefficient and thermal conductivity can be tuned. However, the best performing TBC materials are usually made with rare earths, therefore increasing the cost of the final materials and lowering their industrial appeal. Consequently, another goal is to decrease the cost of HEOs for TBC applications by using cheaper and more widely available elements, such as transition metals.
The high entropy approach is also promising to increase ionic conductivity in oxide- and sulfide-based solid electrolytes for lithium ion batteries by introducing disorder into the rigid host lattice and affecting the dynamics and mobility of the ion species.

[1]Rost, C. M. et al. Entropy-Stabilized Oxides. *Nat Commun* 2015, *6* (1), 1–8.

Prof.ssa Silvia Gross
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