Master Internship

Title	**Prediction of multivalent high entropy oxides**
Location	Laboratoire PMC – Ecole Polytechnique – Route de Saclay – 91128 Palaiseau
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Group website	https://pmc.polytechnique.fr/spip.php?article623&lang=en
Starting date	Spring 2026

Discovery of new materials with interesting properties is traditionally driven by intuition, chemical substitutions, and serendipitous discoveries. Recently, technology giants such as Google and Microsoft are using large databases, generative machine learning, and autonomous labs to accelerate this process, but the experimental realization of the computational predictions often fail because disorder is widespread in real materials[1]. In this project, the student will predict synthesizable and disordered materials using model parameters from density functional theory (DFT). Long-term, the predictions will be verified experimentally through synthesis attempts using solid state synthesis and structural characterization using x-ray diffraction.

The target materials are multivalent high entropy oxides (HEOs). HEOs are heavily disordered yet crystalline oxides where five or more cations share one lattice site in roughly equal amounts[2]. Oxides with heterogeneous cation valences can be realized as long as the total charge balance is preserved. Specifically, we will build on an existing approach where DFT is used to estimate mixing enthalpy and expand the methodology to account for multiple valences[3]. Candidates with background and/or interest in computational methods for material science, inorganic chemistry, or condensed matter physics are welcome to apply. *This internship can be continued as a PhD thesis.*

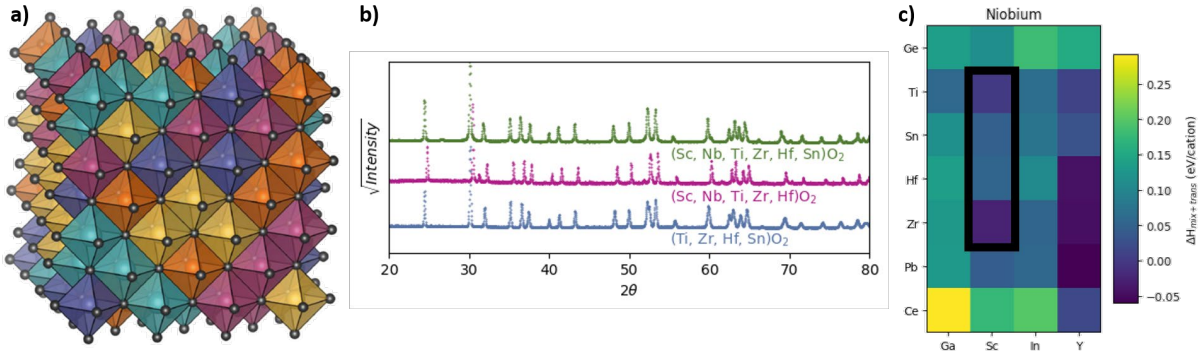

Figure: a) Visualization of a high entropy oxide b) X-ray diffractograms showing successful synthesis of a few new compounds (Sc, Nb, Ti, Zr, Hf)O_2 and (Sc, Nb, Ti, Zr, Hf, Sn)O_2 together with the previously reported (Ti, Zr, Hf, Sn)O_2. All elements in parenthesis are present in equimolar amounts. c) The color map indicates calculated mixing enthalpies for a mixture of three elements (the tetravalent on the y-axis, the trivalent on the x-axis, and the pentavalent element always Nb). A lower mixing enthalpy corresponds to higher likelihood of synthesizability. The black box indicates the chemical space for the successful syntheses in b).

Techniques to be used: Density functional theory (primarily), solid-state synthesis, x-ray diffraction

[1] Cheetham, A. K. et al. *Chem Mater* 36, 3490–3495 (2024) DOI: 10.1021/acs.chemmater.4c00643

[2] Aamlid, S. S. et al. *J Am Chem Soc* 145, 5991–6006 (2023) DOI: 10.1021/jacs.2c11608

[3] Aamlid, S. S. et al. *Commun Mater* 4, 1–11 (2023) DOI: 10.1038/s43246-023-00372-5