Offre de thèse

Nouveaux matériaux supraconducteurs, magnétiques et pour batteries aux ions-fluorure par fluoration topotactique d'intermétalliques

Topotactic fluorination of intermetallics to get novel superconducting, magnetic and fluoride-ion-battery materials

Very recently, a novel synthesis route, implementing the topotactic fluorination of intermetallics for the first time, has allowed preparing new materials for electronics and energy [1].This work opens up a considerable field of investigation in the world of intermetallics, fluorides and more generally in solid-state chemistry and physics.
The objective of the PhD work is to identify new inorganic compositions using this topotactic fluorination of intermetallic compounds and to correlate the structural features to the electronic, magnetic and ionic properties of such solids. For instance, starting with LaFeSi silicide, non-stoichiometric $LaFeSiF_x$ fluoride-silicide ($0.09 < x < 0.85$) which exhibits superconducting behavior, have been synthesized and characterized at ICMCB (Bordeaux) [1].
We will focus on rare earth and transition metal based silicides (where we have a strong experience in the field of synthesis, reactivity and crystal structures), containing interstitial voids (tetrahedral, octahedral, etc…) that are susceptible to accommodate fluorine atoms. We expect the emergence of new physical properties because of their unique chemical bonding, i.e., ionic bonding induced by fluorine in some parts of the structural building blocks and metallo-covalent bonding in other parts of the frameworks.
To achieve the topotactic fluorination of intermetallic precursors whilst avoiding chemical decomposition, the PhD student will use octafluorocyclobutane, C_4F_8 , as gas phase (managed by E. Durand) based on our positive results obtained on LaFeSi and LaScSi silicides (in *collaboration with A. Demourgues and E. Gaudin*). The PhD student will determine and optimize the conditions of fluorination. Alternatively, she/he will also consider other reactants such as fluorinated polymers (PTFE) to reach different F contents (determined by chemical F^- titration using specific electrode). The PhD student will mainly characterize samples by XRD, XPS to determine the structural features and chemical bondings respectively. Local probe such as MAS-NMR and Mossbauer spectroscopies are also available at ICMCB to get information about the local environments and valence states. Resistivity and magnetization measurements will contribute to determine their new physical properties (*collaboration with B. Vignolle*). To test the cycling performance of these new materials used as electrodes for fluoride shuttle-battery, exhibiting mixed ionic and electronic conductivity, a *collaboration with Pr O. Clemens* (University of Stuttgart, DE) is already engaged.

We are looking for a candidate with a master degree in solid-state chemistry (materials sciences or physical chemistry) or with an engineer diploma in chemistry and physics, motivated by the exploratory research of novel materials.
Beginning of the thesis: September 2022

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[1] "***Topotactic fluorination of intermetallics as a route towards quantum materials",*** J-B. Vaney, B. Vignolle, A. Demourgues, E. Gaudin, E. Durand, F. Bernardini, A. Cano, S. Tencé, Nature Comm., 13, 1462 (2022), https://doi.org/10.1038/s41467-022-29043-8