2020 HGF – OCPC – Programme

for the involvement of postdocs in bilateral collaboration projects

Title of the project:

Exploring new electronic phase transition types in novel perovskite compounds

Helmholtz Centre, division/group:

Deutsches Elektronen-Synchrotron – Photon Science - FS-PETRA-D / P02.1

Project leader:

Dr. Martin Etter

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Department/Group: (at the Helmholtz centre or Institute)

FS-PETRA-D / P02.1

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Description of the project (max. 1 page)**:**

Quadruple perovskites (also known as A-site ordered perovskites, general formula AA'3B4O12) exhibit a rich field of fascinating temperature and/or pressure driven electronic phase transition effects (e.g. inter-site charge transfer, charge disproportionation, charge ordering etc.). These phase transitions are usually accompanied by changes in the symmetry of the crystal structure and changes in the macroscopic properties like the magnetization and/or the resistivity, which makes this material class an interesting candidate for the development of new types of sensor devices.

In the last two decades, several different quadruple perovskites were synthesized under high pressure/high temperature conditions with mainly incorporating 3d transition metals on the B-site. Many of the published studies showed, that the choice of the combination of metallic A-cation and 3d metal transition B-site cation is fundamental in determining the final electronic transition effect.

Although the choice of the 3d metal transition cation seems to be essential for the type of the electronic transition, researchers have so far ignored to incorporate heavier elements like the 4d and 5d transition metals on the B-site. This is insofar remarkable, since spin-orbit coupling effects become much stronger in 4d and especially 5d transition metals and therefore it can be assumed that this would lead to unexpected behaviour with possibly new types of electronic phase transitions in quadruple perovskites and subsequent to new types of sensor devices.

For this project, we are seeking for a highly motivated candidate, who is able to work independently on the synthesis of these compounds, which includes weighing of educts, synthesizing precursors by solid state synthesis methods and the assembly and disassembly of the required high pressure environment for a large volume press (LVP) (latter mentioned point can be learned on-site). Since the access to the Large Volume Press is on a collaborative basis, the candidate should be aware that synthesis can only be performed in certain time slots. After the high pressure synthesis, the samples have to be characterized by standard methods, like Microscopy techniques, Scanning Electron Microscope and mainly ambient and temperature dependent Laboratory and Synchrotron Powder X-ray Diffraction.

The project involves a first investigative phase, where principal pressure and temperature parameters have to be defined for the synthesis at the LVP by re-synthesizing already known Quadruple Perovskites. In a second phase, new perovskites will be synthesized incorporating 5d cations. These synthesis processes have then to be optimized, in order to achieve phase pure materials for electric and magnetic characterization techniques. All results have to be published in renowned scientific journals.

The candidate is also encouraged to develop further own scientific ideas and establish collaborations across the DESY center.

Description of existing or sought Chinese collaboration partner institute (max. half page)**:**

Not existing yet

Required qualification of the post-doc:

- PhD in Chemistry, Material Science, Geo-Chemistry or Physics
- Experience with solid state synthesis experiments and chemistry lab work is mandatory. Experience in powder X-ray diffraction techniques (Rietveld refinements) and crystallography are also required. Further experience with high pressure presses would be an advantage.
- Additional skills in standard sample characterization (microscope, scanning electron microscope, X-ray absorption spectroscopy, electric resistivity measurements, measurements of magnetic properties, etc.) would be an advantage
- Language requirement: English fluent in spoken and written language. Knowledge of German language would be good, but is not required. German courses are offered by DESY if there is interest.