Institute for Materials Science
Universität Stuttgart

TECHNISCHE UNIVERSITÄT DARMSTADT

FLAIR

4th of April 2023, 2 pm

Seminar Room 2S02
Heisenbergstr. 3
Stuttgart

Link to WebEx

MIXED-CONDUCTING PEROVSKITES: EFFECT OF ELECTRONIC STRUCTURE ON DEFECTS (PROTONS)

Dr. Rotraut Merkle

MPI für Festkörperforschung, Stuttgart

Abstract:

Triple conducting oxides containing mobile oxygen vacancies, protons, and electronic defects are key functional materials, e.g. as cathode for protonic ceramic fuel cells where the protonic conductivity is decisive to activate the whole cathode surface for the oxygen reduction reaction. Some proton conductivity may be present also in oxides not originally intended as proton conductors, such as memristor materials.

Triple conducting perovskites such as $BaFeO_{3-\delta}$ typically show lower degrees of hydration than $Ba(Ce,Zr,Y)O_{3-z}$ electrolytes, and deviate from ideally dilute behavior.[1,2] The reasons are elucidated from a combination of experiments (thermogravimetry, x-ray absorption spectroscopy XAS) and density functional theory (DFT) calculations.[3,4] DFT results confirm the importance of Fe-O covalency for the materials properties. Electron holes are largely found in oxygen states and thus strongly affect the oxidation as well as hydration reaction. The transition from electrolyte-type to mixed conductors will be discussed on the example of the $Ba(Zr,Fe,Y)O_{3-\delta}$ solid solution. Moderate Fe contents in the range of 10% already strongly decrease the hydration, which can be related to changes in the electronic density of states.

[1] R. Zohourian, R. Merkle, G. Raimondi, J. Maier, Adv. Funct. Mater. 28 (2018) 1801241.

[2] R. Merkle, M.F. Hoedl, G. Raimondi, R. Zohourian, J. Maier, Ann. Rev. Mater. Res. 51 (2021) 461.

[3] G. Raimondi, F. Giannici, A . Longo, R. Merkle, A. Chiara, M.F. Hoedl, A. Martorana, J. Maier, Chem. Mater. 32 (2020) 8502.

[4] M.F. Hoedl, D. Gryaznov, R. Merkle, E.A. Kotomin, J. Maier, J. Phys. Chem. C 124 (2020) 11780.

Host: Prof. Dr. Oliver Clemens