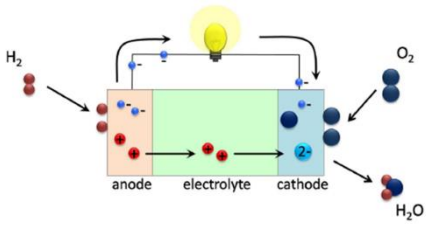
Master thesis project in Computational Physics

H/D isotope effect in proton conducting oxides

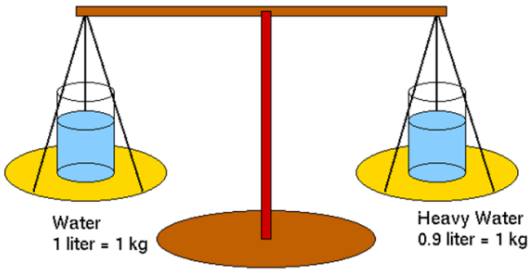
The aim with the project is to investigate possible isotope effects in the hydration of oxides.

Proton conducting oxides have a great potential to contribute to improved and efficient fuel cells, electrolysers and hydrogen separation membranes. Besides conducting protons, the oxides may however conduct also other ions, electrons and holes. For applications it is crucial to understand and control the type of charge species that conduct the current.

It is very difficult to determine the concentration of electronic holes. In a clever experiment Sossina Haile at Caltech used both regular and heavy water when hydrating an oxide [Y. Yamazaki *et al.*, Viewpoint paper, Scripta Materialia 65, 102 (2011)]. By measuring the weight change and making use of the difference in mass between hydrogen and deuterium she could determine the concentration of electronic holes created in the hydration process. She found a surprisingly large concentration of holes and claimed that one has to re-evaluate the thermodynamic characteristics of these types of materials.



However, the experimental analysis is based on the critical assumption that the equilibrium constant for hydration is identical under regular and heavy water uptake. This is not obvious and not known. To compute the equilibrium constant the temperature dependence of the free energy of an acceptor doped oxides with and without protons/deuterons has to be determined.



In the project you will combine theory and computations, and get training in modeling and analyzing complex processes in materials.

More precisely you should: i) set up a theoretical model for the hydration process with regular and heavy water. ii) compute, using density functional theory (DFT), relevant properties needed for the evaluation of the free energy. iii) use this information to determine the hydration constants for regular and heavy water. iv) clarify if the claim by Sossina Haile is correct.

The project is suitable as a 30 hp master project, for one or two students. Useful background courses are Thermodynamics and statistical mechanics, Computational Physics and Computational Materials Physics. You should have an interest in modeling and a good background in combining theory and computations.

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