Advertisement of
Two Master Thesis Projects

Universität Stuttgart

Advanced Understanding of Materials for Fluoride Ion Batteries: A theoretical study

Fluoride Ion Batteries (FIBs) are all solid state batteries which are based on the use of solid electrolytes [1]. Such batteries were first established using conversion based electrode materials (conversion from a metal to the respective metal fluoride and vice versa) [2]. A current aim of the group of Prof. Clemens is to build FIBs based on intercalation electrodes, with the best suitable candidates so far crystallizing within the Ruddlesden-Popper (RP) type structure [3].

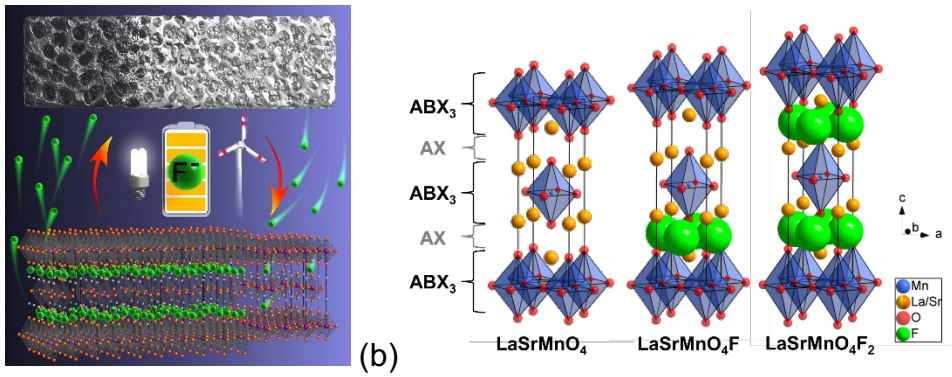

Fig. 1. (a) Scheme of Fluoride Ion Battery. (b) $LaSrMnO_4$ and its fluorinated phases – potential candidates for high voltage cathodes for Fluoride Ion Batteries.

Though experimental findings have advanced over the last years, only little is understood on various aspects within this battery systems in many aspects: What are the diffusion pathways within the various electrode and electrolyte materials and how large are the intrinsic activation energies? Is there anion reordering of oxide and fluoride ions occurring on charging/discharging of the battery? What is the influence of the redox inert cation on stabilizing/destabilizing the host structure? What are the theoretically predicted potentials and stability windows of the different materials?

These questions will be addressed using theoretical approaches (DFT, molecular dynamics) within the master theses advertised here.

References

[1] M. Anji Reddy, M. Fichtner, *J. Mater. Chem.* **2011**, *21*, 17059-17062.

[2] a) C. Rongeat, M. Anji Reddy, T. Diemant, R. J. Behm, M. Fichtner, *J. Mater. Chem. A* **2014**, *2*, 20861-20872; b) C. Rongeat, M. Anji Reddy, R. Witter, M. Fichtner, *ACS Applied Materials & Interfaces* **2014**, *6*, 2103-2110.

[3] a) O. Clemens, C. Rongeat, M. A. Reddy, A. Giehr, M. Fichtner, H. Hahn, *Dalton Trans.* **2014**, *43*, 15771-15778; b) M. A. Nowroozi, K. Wissel, J. Rohrer, A. R. Munnangi, O. Clemens, *Chem. Mater.* **2017**, *29*, 3441-3453.

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