PHYSIKALISCHES KOLLOQUIUM

AM 16. OKTOBER 2017 UM 17 UHR C.T.

IM GROßEN HÖRSAAL

UNDERSTANDING AND MANIPULATION OF IONIC SYSTEMS …!

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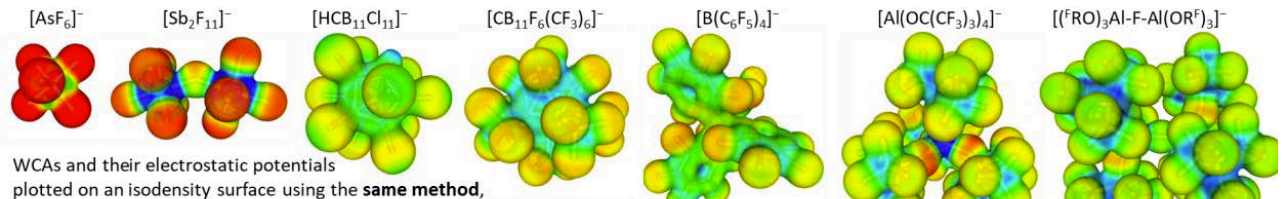
Ionic Systems: Over the last 20 years we have been involved in the design, understanding and application of Ionic Systems, i.e. matter that is predominantly built from charged ions. Our focus hereby lies on systems, in which cation and anion interact as weakly as possible. This is relevant to study reactive ions that for example were first detected in the gas phase of a mass spectrometer in the condensed phases, but is of equal importance, if one needs to design a very effective electrolyte for a battery system. The lecture will give an extended overview onto the principles underlying Ionic Systems and describe selected examples from own work.

Weakly Coordinating Anions (WCAs): One ingredient in the Ionic Systems described is a WCA. In principle those are large to very large almost spherical and preferably -1 charged chemically robust entities, the exterior of which is often terminated by fluorine to create a “non-sticky Teflon-effect”. This is mainly due to the low polarizability of element-fluorine bonds and the capability of fluorine to effectively delocalize the negative charges. The figure below gives an overview on the evolution of such WCAs.



WCAs and their electrostatic potentials plotted on an isodensity surface using the **same method**, **basis set** and **cut off** (PBE0/TZVPP). Red color indicates accumulation of negatively charged areas, neutral areas are greenish and blue areas are positive polarized.

The Ionic Systems constituted by these WCAs will include:

Gas Phase Cations in the condensed phase? The concept of *Pseudo Gas Phase Conditions* will be delineated and established with examples.
Ionic Liquids (ILs) go ideal: ILs with the [Al(ORF)4]– WCA show almost ideal behavior and are prototypes for electrolytes.
Electrolytes for Battery Systems: We present the understanding of the failure mechanism of a Lithium-Sulfur battery and delineate a resolution based on a WCA electrolyte.