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Exploring ionic liquids and solar water splitting catalysis via high-performance ab initio molecular dynamics

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Ionic liquids receive more and more attention due to their potential applications as, for instance, electrolytes and green solvents. Being composed of charged entities, they exhibit favorable properties of high interest for use in laboratories and industry. In order to study their complex behavior, dynamic *ab initio* calculations are indispensable. The same is true for the understanding of water splitting catalysts in solution. Detailed analysis of their catalytic functioning and the factors determining their efficiency are a prerequisite for the design of more efficient catalysts. We present our recent research for the in-depth study of ionic liquids and water splitting catalysis using forefront computational methods such as high-performance *ab initio* molecular dynamics.

Biography

Sandra Luber received her MSc and PhD degree from ETH Zurich in 2007 and 2009, respectively. After Post-doctoral studies at Biozentrum of the University of Basel (2010) and Yale University (2010-2011), she joined BASF SE in 2012 followed by a position as Project Group Leader at University of Zurich. Currently, she is SNSF Professor at the University of Zurich. She is a recipient of many awards that include the ETH medal for an outstanding PhD thesis, the IBM research prize for computer modeling and simulations in Chemistry, Biology, and Materials, and the Clara Immerwahr Award 2017.

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