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Efficient cubane catalysts for artificial water-splitting

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Solar energy is an inexhaustible energy source for a long-term solution to the global energy consumption. The storage of large amounts of light energy can be achieved by conversion into chemical energy saved in biomass. Artificial photosynthesis permits the splitting of water into dihydrogen and dioxygen and is therefore a sustainable strategy to meet the increasing worldwide need for clean energy. This requires the development of high-performance water reduction and water-oxidation catalysts (WOCs) that can be combined to an overall artificial photocatalytic water-splitting system. Very recently, the first Co (II)-based cubane WOCs have been presented. These WOCs excel through hitherto unprecedented structural analogies to the oxygen-evolving complex of nature's photosystem II. We study their structure and activity by means of density functional theory (DFT) in combination with innovative DFT-based molecular dynamics. I will give an overview about our recent results for the design of efficient cubane-type catalysts.

Biography

Sandra Luber received her MSc and PhD degree from ETH Zurich in 2007 and 2009 respectively. After postdoctoral studies at Biozentrum of the University of Basel (2010) and Yale University (2010-2011), she joined BASF SE in 2012. Currently, she works on her Postdoctoral lecturing qualification (Habilitation thesis) at the University of Zurich. Her awards include the ETH medal for an outstanding PhD thesis as well as the IBM Research Prize for Computer Modelling and Simulations in Chemistry, Biology, and Materials Science.

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