Nagoya University

IGER NAGOYA UNIVERSITY **Platform:** Nano/Energy

RCMS Research Center for Materials Science, Nagoya University

Theoretical Chemistry Colloquium

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RCMS, 2nd floor, Chemistry Gallery

Electronic Structure of Polyoxometalates: From the Nucleation of Small Polyoxotungstates to the Properties of Large Anions

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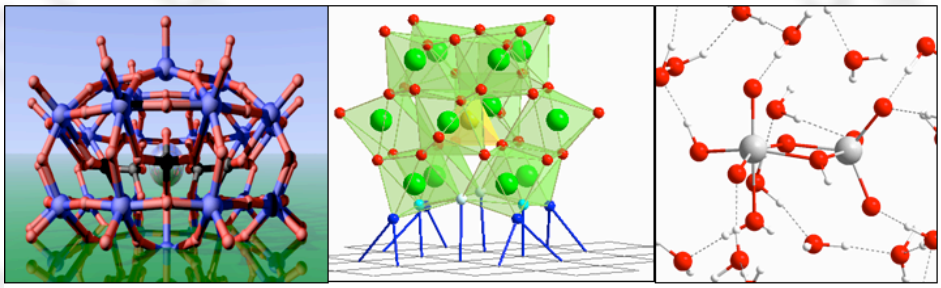

Abstract: *During the last fifteen years our group has been interested in the characterization of the electronic properties of polyoxometalates (molecular metal oxides) by means of theoretical methods. We have demonstrated that the redox and structural properties of typical polyoxotungstates or polyoxomolybdates such as the Keggin ($XM_{12}O_{40}^{m-}$), Well-Dawson ($X_2M_{18}O_{62}^{n-}$) and Preyssler ($NaP_5W_{30}O_{110}^{q-}$) anions can be reproduced and rationalized by means of DFT methods using the COSMO approach to model the solution.[1-3] We report here some of the most recent results of the group on the electronic properties of fully oxidized and reduced polyoxometalates. In particular, we will discuss the redox properties of polyoxotungstates, the origin of alternating bond distortions in polyoxomolybdates, the nucleation mechanism in the formation of polyoxotungstates[4] and the modelling of the interaction between polyoxometalates and metal surfaces.[5]*

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