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DFT Simulation of Complex Reaction Networks: New Insights into the Speciation and Formation of Polyoxometalates

In recent years our group has been working in the development of a new computational methodology, which we called POMSimulator,[1] to simulate the complex multi-species multi-equilibria taking place in the self-assembly processes leading to polyoxometalates. POMSimulator comprises automated workflows that rely exclusively on DFT-based results, and has been successfully applied to Mo, W, V, Nb and Ta isopolyoxometalates (IPAs). [2,3] The reaction networks can be applied to perform very long multi-time scale kinetic simulations on the formation of isopolyoxotungstanates, [4] what led to the discovery of a reaction mechanism that transforms the kinetic product {W12} in the thermodynamic product {W10}. We released recently the first open-source version of the code. [5] On the other hand, heteropolyoxoanions (HPAs) introduce far more complexity. We carried out a statistical analysis of the massive amounts of data produced by POMSimulator to reduce the reliance of the method on experimental formation constants. [6,7] More recently, we combined the predictions of our method with new Z-Ray total scattering data to investigate polyoxomolibdates speciation under hydrothermal conditions.[8]

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