

# From Lindqvist Anions to Giant Structures: DFT Studies of Polyoxometalates

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The continuous progress of computers in general, and quantum chemistry software in particular, has enabled a number of topics in polyoxometalate (POM) chemistry to be theoretically studied. In this communication, we summarize some of the most recent quantum chemistry studies carried out by our group on POMs.

After discussing the steps involved in the formation of a  $W_6O_{19}^{2-}$  anion, we will show that redox and basicity properties of polyoxotungstates as well as the reactivity of functionalized POMs can be easily rationalized from DFT calculations. Ion exchange in POMs and the electronic properties of some *large* polyoxomolybdates will be also discussed.