Prediction of first-order nonlinear optical properties of Anderson polyoxometalate derivatives

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Polyoxometalates (POMs) are metal-oxygen oxo-clusters with a large variety of sizes and shapes. The most known POMs types are: Wells-Dawson, Keggin, Anderson, and Lindkvist types. They are largely studied for their application in different fields such as: catalysis, materials science, and medicine.

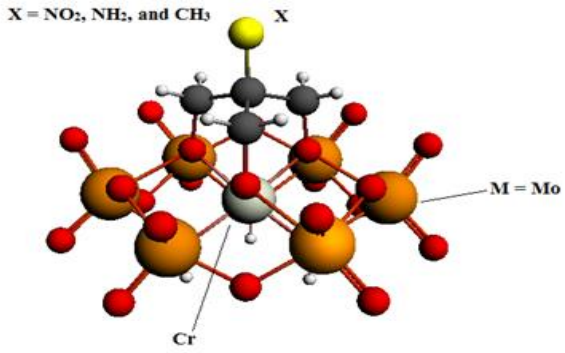

Figure. Ball and sticks representation of Anderson structure and its derivatives

POMs have been largely investigated for their chemical and physical properties: redox, photovoltaic applications, chemical reactivity, nonlinear optical properties … etc. In order to establish the structure-property relationship, we proposed in this work to study a set of Anderson cluster's derivatives $[X\text{-}C(CH_2O)_3CrMo_6(OH)_3O_{18}]^{3-}$ (X = NO_2, NH_2, and CH_3) and substituted Polyoxometalates $[CrMo_6O_{24}]^{3-}$. The first-order hyperpolarizabilities, the partial density of states PDOS, and the electronic spectrum of those clusters have been evaluated using the density functional theory (DFT) and the time-dependent DFT (TD-DFT) methods.