Interactions of Polyoxometalates with Carbon Nanotubes and Surfaces

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Polyoxometalates (POMs) chemistry is a key emerging area that underpins applications in a variety of disciplines including catalysis, material science, biology and medicine.[1] An extensive range of physical and chemical properties of POMs makes them ideal building blocks for the development of new materials and functional devices. The surface patterning of POMs could also be an important step towards gaining spatial control. However POMs have rarely been covalently anchored to surfaces.[1]

Meanwhile, Sloan *et al* has recently imaged with atomic resolution Tungsten-based POM ions, including the $[W_6O_{19}]^{2-}$ Lindqvist ion and the $[\gamma\text{-}SiW_{10}O_{36}]^{8-}$ lacunary Keggin ion, not only within double walled carbon nanotubes and but also on monolayer graphene oxide (GO) surface.[2-4] In order to understand the nature and the strength of binding we use density functional theory (DFT) to calculate the structure and electronic properties of POMs encapsulated within carbon nanotubes and interacting with GO surface. This presentation will discuss the most récent theoretical results including electronic structure, binding energy and charge distribution in these composites.

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