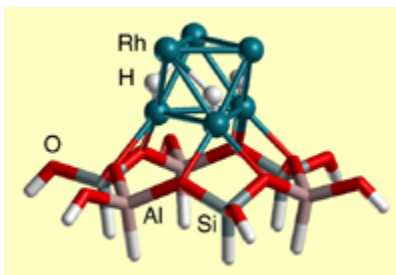


Zeolites



Oxide-supported transition metal particles are widely used as catalysts and as components of sensors, photovoltaic cells, and magnetic recording devices. Knowledge at the atomic level about the interactions of metal clusters with oxide supports is still far too scarce which notably hinders technological applications of these advanced materials. The group carries out systematic electronic structure calculations on these systems to fill that knowledge gap. A spectacular result, obtained for Ir_4 clusters in zeolites and substantiated for Rh_6 species, is that chemically prepared supported metal particles are not entirely ligand-free, but contain attached light atoms.

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