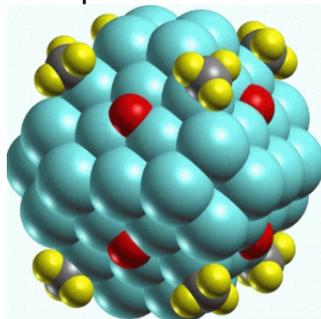


# Electronic structure of metal clusters

## Transition Metal Clusters and Cluster Compounds



Clusters constitute an intermediate state of matter between molecules and solids. Physical and chemical properties of clusters, which range from sub-nanometer to about 1 micrometer, are size-dependent and thus tunable. This fact is of particular interest in materials science, catalysis and other fields of applied sciences such as nanoelectronics. The main goal of our research is to determine chemical properties, reactivity, composition and structure of metal clusters. We apply density functional calculations in several topics of cluster science: (1) Small isolated transition metal clusters and their compounds, which serve as reference systems in heterogeneous catalysis. (2) Studies of unique properties of isolated clusters in comparison to supported species. (3) Larger transition metal clusters, which have successfully been shown to act as reliable models for studying chemical reactions on solid state surfaces. (4) Ligand stabilized species like nickel carbonyl and gold thiolate clusters - because of their usefulness as flexible and versatile building blocks in nanochemistry.

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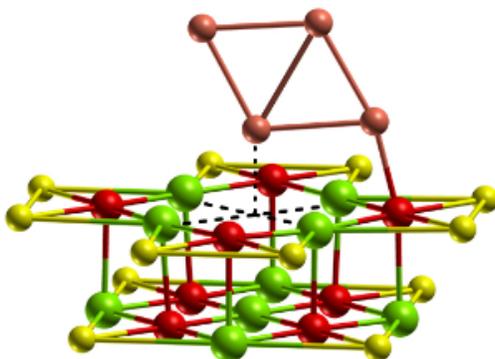
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## Oxide-Supported Transition Metal Particles



Systems composed of metal particles or metal films supported on an oxide are of immediate relevance for many applications, one of which is heterogeneous catalysis. Several years ago we initiated systematic computational studies of small  $\alpha$ -metal particles deposited on the touchstone oxide support MgO using density functional (DF) cluster models. [6] More recently we went on to apply an advanced cluster embedding method (EPE), which is one of the most accurate cluster model methods currently available, to investigate systematically the adsorption of 17 single  $\alpha$ -metal atoms across the periodic table with the regular  $O^{2-}$  sites on MgO(001) terraces [7] as well as with  $F_s$  and  $F_s^+$  oxygen vacancies. [8] These studies showed that, at variance with general belief, some  $\alpha$ -metal atoms do not form stronger bound adsorption complexes with F-type surface defects than with regular sites and that metal atoms in  $M_1/F_s$  complexes accumulate considerable amount of electron density, which governs the trend of the adsorption energies. We extended our studies of atoms on MgO(001) to larger metal particles. For instance, we addressed interactions of coinage metal dimers, trimers and tetramers with regular sites and O-vacancies on MgO(001). [9] We have developed a time-dependent DFT tool in ParaGauss, which allows to calculate optical transitions in adsorbed systems. These transitions are believed to be characteristic of the adsorption species size, morphology, adsorption site and adsorption geometry. Thus, theory can complement experimental studies in the interpretation of the results obtained for complex systems.

See also a related topic [Zeolites](#)

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