Mini-symposium C10
Recent advances in the science of clusters

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C10-01 Keynote
Predicting Properties of Clusters, Molecules and Nanocrystals Interacting with Static and Dynamic Fields
James R. Chelikowsky
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Recent numerical methods will be discussed that can be used to predict the response of localized systems such as nanocrystals, clusters and molecules to applied fields. Our computational methods are based on pseudopotentials constructed within density functional theory, and employed in real space. Real space methods possess a number of advantages shared by methods employing plane waves. For example, they are easy to implement and one parameter controls convergence. However, unlike plane wave methods, real space methods minimize global communications when implemented on parallel platforms and are amenable to new algorithms for fast eigensolvers. Moreover, they can readily handle charged systems. As such, they are ideally suited for confined systems. I will illustrate these real space methods and other methods for a number of applications, which will include the polarizability of Na clusters, the vibrational Stark shift in organic molecules, the photoemission spectra of silicon and titania clusters, the Stokes shift in silicon clusters, and the Raman spectra of both intrinsic and doped nanocrystals.

C10-02 Invited
Exploring and understanding the potential energy landscape of clusters
Stefan Goedecker
University of Basel Switzerland

Minima hopping based methods will be presented that allow to find the characteristic stationary points of the potential energy surface, namely minima and saddle points, in an efficient way on the density functional level. Based on this, methods will then be discussed that allow to characterize not only the structural but also the dynamic properties of clusters from information about the potential energy landscape. The different behavior of clusters based on such a characterization will be illustrated for carbon, boron and gold clusters.

C10-03 Invited
Determining and Analyzing the Properties of Nanoparticles
Michael Springborg
Physical and Theoretical Chemistry, University of Saarland, 66123 Saarbrücken, Germany

One of the big challenges facing theoretical studies of nanoparticles is to determine the structure of the global total-energy minimum. During the last couple of decades more different approaches have been proposed for tackling this problem and also applied to various systems in combination with more or less accurate descriptions of the total energy as a function of structure. As result of such calculations one obtains first of all the nuclear coordinates and the total energies as functions of the size of the clusters. Another challenge is then to extract chemically or physically relevant information from this often very large amount of information.

In this presentation we give examples from our own work on the unbiased determination of the structure of different types of clusters. We have used different structure-optimization methods as well as approximate total-energy methods, and shall put special emphasis on the analysis of the results. This includes the identification of particularly stable clusters as well as the structural shape and similarity with various types of reference structures.

As examples we consider isolated metal clusters and metal clusters deposited or grown on metal surfaces. Also semiconductor clusters with one or more types of atoms shall be treated.

C10-04 Invited
Magnetism of clusters and molecules
Olle Eriksson
Department of Physics and Astronomy, Uppsala University, Box-516, 75120, Uppsala, SWEDEN

In this talk I will present theoretical aspects of magnetism of selected molecules and clusters. This will involve transition metal containing porphyrins and phthalocyanins, as well as rare-earth based clusters. Theoretical considerations based on various forms of density functional theory will be discussed, and in particular a comparison will be made between experimental data and theory, as concerns spin and orbital magnetism as well as the spin-dipole contribution of XMCD experiments. In addition, correlation effects within dynamical mean field theory will be discussed, and a comparison between correlated and uncorrelated theory will be made.

C10-05 Invited
Chiral Spin Textures at Transition Metal Surfaces
Stefan Blügel
Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

I will talk about the chiral magnetism of transition-metal atoms in small clusters at surfaces experiencing magnetism in a structure inversion asymmetric environment. The presence of magnetism and spin-orbit interaction of atoms in such an environment gives rise to a chiral magnetic interaction, known as the Dzyaloshinskii-Moriya interaction (DMI). In the context of thin magnetic transition-metal films or clusters this interaction has been overlooked for more than 30 years. However, the recent observations of new magnetic phases as in an atomic monolayer of Mn on a W(110) substrate [1], whose magnetic ground state is a frozen cycloid of unique rotational sense, or of a chiral non-trivial two-dimensional magnetic structure, that is interpreted as nano-Skyrmeon lattice [2], proved its impact and has opened a completely new vista of low-dimensional magnetism. Maybe not surprisingly, little is known about the DMI in low-dimensional systems, such as films, chains, clusters or adatoms, neither in terms what determines its strength nor sign, and a recent model developed by us for zigzag chains [3] indicates the dependence of the sign and strength of the DMI on the electronic structure is non-trivial.


C10-06
F_{ex} (n = 1–6) clusters chemisorbed on vacancy defects in graphene: Stability, spin-dipole moment, and magnetic anisotropy.
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In this talk, we have studied the chemical and magnetic interactions of Fe_{n} (n = 1–6) clusters with vacancy defects (monovacancy to
correlated vacancies with six missing C atoms) in a graphene sheet by \textit{ab initio} density functional calculations combined with Hubbard U corrections for correlated Fe-d electrons. It is found that the formation of correlated vacancy is facilitated and the vacancy formation energies are lowered in the presence of Fe, indicating an easier destruction of the graphene sheet. Due to strong chemical interactions between Fe clusters and vacancies, a complex distribution of magnetic moments appear on the distorted Fe clusters which results in reduced averaged magnetic moments compared to the free clusters. In addition to that, we have calculated spin-dipole moments and magnetic anisotropy energies. The calculated spin-dipole moments arising from anisotropic spin density distributions vary between positive and negative values, yielding increased or decreased effective moments. Depending on the cluster geometry, the easy axis of magnetization of the Fe clusters shows in-plane or out-of-plane behavior.


\textbf{C10-07}

Theoretical Studies of Thermodynamic Properties of Clusters

\textit{ Yi Dong, Michael Springborg}

\textit{Physical and Theoretical Chemistry, University of Saarland, 66123 Saarbrücken, Germany}

As an extension of our earlier study on the structural properties of the clusters, a recently developed method to calculate the low-temperature vibrational heat capacities of clusters shall be presented. Subsequently, it shall be applied to Au\(_n\), Na\(_n\), Si\(_n\), Ge\(_n\), and Si\(_n\)Ge\(_n\) clusters. Our approach does not attempt to identify phase transitions but focuses on the low temperature behaviour, we find that the vibrational heat capacity of the clusters is strongly size dependent at low temperatures, and for the smallest clusters. This becomes less pronounced when the size and/or temperature increases. An interesting observation is that some structures have a particularly large vibrational heat capacity at low temperatures, and that is not correlated with particularly high or low stability of those clusters.

\textbf{C10-08 Invited}

Novel nanostructures of boron: Bowls, rings, tubes, cages, and sheets

\textit{Vijay Kumar}

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Boron is just before carbon in the periodic table and there has been much interest to explore if it can have nanostructures similar to fullerenes and nanotubes of carbon. However, boron is electron deficient and there is preference for 3-center bonding. This led to theoretical studies [1] of B\(_{10}\) fullerene structure in which 20 hexagons of C\(_{12}\) like structure have a boron atom at the center. However, later lower energy structures have been obtained. Recently there are developments of the realization of fullerene-like structure of B\(_{10}\) and a bowl shaped structure of B\(_{16}\). We shall briefly review these developments and present our new results on B\(_{10}\) and several other sizes [2] for which we have studied bowl, rings, tubular, and cage-like structures. We shall discuss the importance of hexagonal holes and chains in the stability of the boron nanostructures as obtained from \textit{ab initio} calculations and the stability of the quasi-planar bowl-shaped structures in terms of multi-center two-electron bonding. It is found that the binding energy of such quasi-planar structures approaches the value for α-boron sheet.


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\textbf{C10-09 Invited}

Structures and growth behavior of gas-phase and metal-supported boron clusters

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We evaluate the performance of the exchange-correlation functionals of DFT in the energetics of boron clusters using CCSD(T) and MP2 results as benchmark [1]. The PBE, TPSS, TPSSh, and PBE0 functionals are recommended. Using simulated annealing with ab initio molecular dynamics, we have determine the lowest-energy structures of boron clusters with n=26, 28, 30, 32, 68, 74, 80, 101. We find strong competition between different structural motifs (cage, bowl, tube) for medium-sized boron clusters (n=26-32), whereas the large boron clusters such as B\(_{80}\) [2] and B\(_{101}\) [1] prefer core-shell configurations with B12 icosahedral core. We also explore the structures of boron clusters supported on Cu(111) surface and discuss the growth mechanism into monolayer boron sheet [3].


\textbf{C10-10 Invited}

Correlated electronic structures of metalorganic molecules

\textit{Biplab Sanyal}

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A proper theoretical description of electronic structure of the 3d orbitals in the metal centers of functional metalorganics is a challenging problem. In this talk I will demonstrate a method that combines density functional theory and exact diagonalization in a many body approach to study the ground state electronic configuration of an iron porphyrin (FeP) molecule. It will be shown that dynamical correlation effects are important, and FeP is a potential candidate for realizing a spin crossover due to a sublattice balance of crystal field effects, on-site Coulomb repulsion and hybridization between the Fe-d orbitals and ligand N p-states. Moreover, the mechanism of switching between two close lying electronic configurations of Fe-d orbitals is revealed. The generality of the suggested approach and the possibility to properly describe the electronic structure and related low energy physics of the whole class of correlated metal centered metalorganic molecules will be discussed.

\textbf{C10-11}

A computational study of Cu clusters within ferrite Fe matrix on atomic scale

\textit{Lin Zhang}

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Reactor pressure vessel(RPV) steels in nuclear reactors are subjected to neutron irradiation. These produce severe embrittlement, where the embrittlement is characterized by an upward shift in the transition temperature in excess of 300K in some cases. Experimental evidence strongly relates this property change to the occurrence of initially small BCC Cu precipitates in the RPV steels.

While a significant experimental database on the nanometer precipitates and the matrix features exists, a more detailed atomic scale understanding is required to better underpin predictive the irradiation embrittlement of pressure vessels and the alloying behavior in these materials. Therefore, the following important issue will be naturally arisen to understand structural transformation for the Cu small particles within the Fe matrix upon heating.

In the work, molecular dynamics(MD) simulations are presented to study the structural transition of small Cu particles within ferrite Fe matrix at elevated temperature. Upon heating, accompanying with the movement of tagged Cu atoms, the stress changes of the tiny volume elements occupied by the Cu atoms are also demonstrated.