

A 16: Atomic Clusters II

Zeit: Mittwoch 14:00–16:00

Raum: VMP 6 HS-B

Fachvortrag

A 16.1 Mi 14:00 VMP 6 HS-B

Ion and electron emission from Argon clusters in intense femtosecond XUV laser pulses — ●MATHIAS ARBEITER and THOMAS FENNEL — Institute of Physics, University of Rostock, Germany

The ionization dynamics of Argon clusters in ultrashort and intense XUV laser pulses is investigated by molecular dynamics simulation. Corresponding experiments^[1] at FLASH free electron laser at $\lambda = 32$ nm and $\lambda = 13$ nm with intensities of $I \sim 10^{12-14}$ W/cm² have demonstrated the cluster response to be completely different to the behavior observed in the infrared and the VUV regime, where plasma heating processes dominate the laser-cluster coupling. In the XUV regime, in contrast to that, the measured photoemission spectra indicate a series of direct electron emission events in the developing cluster Coulomb field. According to this, nanoplasma formation takes place only if the cluster potential is sufficiently deep to suppress direct electron emission. In our MD analysis we focus on the impact of thermalization and laser heating on the electron and ion emission spectra. Whereas the low-energy tail of the photoemission spectra is severely affected by thermalization for higher intensities, laser heating through inverse Bremsstrahlung turns out to be insignificant^[2]. Methodical details and simulation results will be presented and discussed in comparison with experimental results.

[1] C. Bostedt et al., Phys. Rev. Lett. 100, 133401 (2008)

[2] M. Arbeiter, in preparation

Fachvortrag

A 16.2 Mi 14:30 VMP 6 HS-B

Vibronic coupling and energy transfer on aggregates — ●ALEXANDER EISEL — MPI-PKS Dresden, Finite Systems

Self-organised J-aggregates of dye molecules, known for over 60 years, are emerging as remarkably versatile quantum systems with applications in photography, opto-electronics, solar cells, photo-biology and as supra-molecular fibres [1].

The optical properties and the energy transfer dynamics of such molecular aggregates are strongly affected by internal vibrations of the constituting monomers, which couple to the electronic excitation. Detailed features of the aggregate spectra could be explained using the "coherent exciton scattering" approximation [2].

A new approach based on a non-Markovian Schrödinger equation [3] allows to investigate the influence of a continuous structured phonon bath on the energy transfer and to treat uniformly the transition from coherent to incoherent motion.

[1] T. Kobayashi, (ed.) J-Aggregates, World Scientific, 1996

[2] A. Eisfeld, J. S. Briggs, Chem. Phys. 324, (2006) 376

[3] T. Yu, L. Diosi, N. Gisin, W. Strunz, Phys. Rev. A. 60, (1999) 91

A 16.3 Mi 15:00 VMP 6 HS-B

Electronic and magnetic properties of size selected scandium and manganese doped silicon cluster cations —

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Because of its high abundance in mass spectra and backed by theoretical predictions, VSi_{16}^+ is assumed to be a 'magic' transition metal doped silicon cluster with high symmetry and electronic shell closure. Core level spectroscopy on size-selected clusters in an ion trap recently revealed that TiSi_{16}^+ , VSi_{16}^+ , and CrSi_{16}^+ are indeed highly symmetric cage clusters which can be described in the spherical potential model. Extending our studies to ScSi_{16}^+ and MnSi_{16}^+ , we show that this simple description is no longer valid if the cage geometry and the number of valence electrons deviate strongly from the ideal situation in VSi_{16}^+ . Instead, the Mn 2p X-ray absorption spectrum indicates that MnSi_{14}^+ is a symmetric cluster with a local d^5 configuration of the Mn atom, pointing at a high spin state. This is the first experimental evidence of a high magnetic moment in transition metal doped semiconductor clusters. We will discuss these results together with electronic properties and reactivities of ScSi_n^+ and MnSi_n^+ clusters.

A 16.4 Mi 15:15 VMP 6 HS-B

Transition metal and silicon 2p photoionization of Ti, V, and Cr doped Si_n^+ cages — ●ANDREAS LANGENBERG¹, MARLENE VOGEL¹, KONSTANTIN HIRSCH¹, PHILIPP KLAR¹, FABIAN LOFINK¹, JÜRGEN PROBST¹, ROBERT RICHTER¹, JOCHEN RITTMANN¹, VICENTE ZAMUDIO-BAYER¹, THOMAS MÖLLER¹, BERND VON ISSENDORFF², and TOBIAS LAU¹ — ¹Technische Universität Berlin, Institut für Optik und Atomare Physik, EW 3-1, Hardenbergstr. 36, 10623 Berlin — ²Albert-Ludwigs-Universität Freiburg, Fakultät für Physik/FMF, Stefan-Meier-Str. 21, 79104 Freiburg

Silicon 2p photoionization spectroscopy of titanium, vanadium, and chromium doped Si_n^+ cages complements X-ray absorption studies at the transition metal 2p edges. While clusters with lower symmetry show broad bands in resonant silicon 2p photoionization, the highly symmetric TiSi_{16}^+ , VSi_{16}^+ , and CrSi_{16}^+ clusters are characterized by a rich line structure in their spectra. This is a further indication of a highly degenerate density of states and electronic shells in these clusters. Furthermore, resonant and direct photoionization channels are associated with different fragmentation patterns at the silicon 2p edge and can be separated *ex post* in ion yield spectra. This gives access to the direct photoionization threshold and even to x-ray photoelectron spectra. Compared to VSi_{15}^+ and VSi_{17}^+ , the direct 2p photoionization threshold of magic VSi_{16}^+ is shifted by approx. 0.7 eV to higher photon energy because of the large HOMO-LUMO gap. We will discuss our recent results with an outlook at valence band photoionization spectroscopy of cationic clusters.

A 16.5 Mi 15:30 VMP 6 HS-B

2p-Photoionisation an freien gröÙenselektierten Silizium-Clustern — ●MARLENE VOGEL¹, KONSTANTIN HIRSCH¹, PHILIPP KLAR¹, ANDREAS LANGENBERG¹, FABIAN LOFINK¹, JÜRGEN PROBST¹, ROBERT RICHTER¹, JOCHEN RITTMANN¹, VICENTE ZAMUDIO-BAYER¹, BERND VON ISSENDORFF², THOMAS MÖLLER¹ und TOBIAS LAU¹ —

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Die Röntgenspektroskopie an freien Clustern stellt aufgrund der niedrigen Targetdichte und des niedrigen Röntgenphotonen-Flusses eine Herausforderung dar. Nun ist es gelungen, Innerschalen-Röntgenspektroskopie an gröÙenselektierten freien Siliziumclustern durchzuführen. Dadurch ist die 2p-Schwelle von freien Siliziumclustern erstmals einer Beobachtung zugänglich.

An gröÙenselektierten Clustern Si_n^+ , $n \geq 5$ wird der Übergang $2p \rightarrow 3d$ und die direkte 2p-Photoionisation im Energiebereich 90 - 115 eV untersucht. Die Spektren zeigen auf deutliche Weise die Entwicklung des Festkörperspektrums aus den Spektren der kleinen Cluster. Darüber hinaus ist durch diese Messungen erstmals die Lage der 2p-Schwelle experimentell zugänglich. Die gröÙenabhängige Änderung dieser Schwelle läÙt sich gut durch das Spiegelladungsprinzip einer Metallkugel beschreiben.

A 16.6 Mi 15:45 VMP 6 HS-B

X-rays reveal high symmetry and electronic shells in transition metal doped silicon clusters — ●JOCHEN RITTMANN¹,

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Incorporation of a transition metal atom leads to a complete geometric rearrangement of silicon clusters. X-ray absorption spectroscopy at the dopant atom 2p edge unravels a high symmetry of TiSi_{16}^+ , VSi_{16}^+ , and CrSi_{16}^+ cages. We show that Ti, V, and Cr adopt the same local electronic structure when embedded into Si_{16} . Our data can be explained within the spherical potential model, where the electronic shell structure of the cage interacts with the dopant atom orbitals of the same character. Charge transfer to the silicon cage leads to a local d^0 configuration of the transition metal dopant, quenching the magnetic moment. Because of its closed electronic shells, VSi_{16}^+ can be described as a spherically aromatic system according to the $2(N+1)^2$ rule. Our findings are further corroborated by the fact that the local

electronic structure of the dopant is unchanged when replacing the Si_{16} cage by Ge_{16} .