

## O 85: Poster Session - Supported Nanoclusters: Structure, Reactions, Catalysis

Time: Wednesday 18:15–20:00

Location: P2/EG

O 85.1 Wed 18:15 P2/EG

**Bottom-up synthesis of free-standing nanocluster arrays supported by carbon** — •TOBIAS HARTL<sup>1</sup>, MORITZ WILL<sup>1</sup>, SOPHIA DELLMANN<sup>1</sup>, DAVOR ČAPETA<sup>2</sup>, VIRGINIA BOIX DE LA CRUZ<sup>3</sup>, RAJENDRA SINGH<sup>4</sup>, DANIEL SCHEINECKER<sup>4</sup>, PAOLO LACOVIG<sup>5</sup>, SILVANO LIZZIT<sup>5</sup>, JANI KOTAKOSKI<sup>4</sup>, JAN KNUDSEN<sup>3</sup>, MARKO KRALJ<sup>2</sup>, THOMAS MICHELY<sup>1</sup>, and PANTELIS BAMPOULIS<sup>1</sup> — <sup>1</sup>University of Cologne — <sup>2</sup>Institute of Physics, Zagreb — <sup>3</sup>MAX IV Laboratory, Lund — <sup>4</sup>University of Vienna — <sup>5</sup>Elettra Synchrotron, Trieste

Cluster superlattices exhibit unique properties stemming from their small size and dimensionality. However, their use in applications is hampered by their low stability when exposed to application relevant conditions, e.g. ambient pressure, high temperature. We succeeded in synthesizing free-standing membranes hosting metal cluster superlattices which are stable at these conditions. We present, in detail, the fabrication process of such membranes. The cluster superlattices are grown on graphene on Ir(111), and subsequently embedded in a few nanometer thick carbon matrix. XPS and STM reveal that the carbon embedding is conformal to the clusters, anchors them to the graphene and greatly improves their thermal and mechanical stability. Removal of the membranes from the Ir(111) substrate by hydrogen bubbling is possible, when a substantial reduction of the graphene-Ir binding is accomplished by annealing at 850 K and intercalation of Eu. Post-removal TEM analysis of the cluster lattice membrane proves that the excellent order of the cluster lattice is maintained in the free-standing membrane.

O 85.2 Wed 18:15 P2/EG

**Hydrogenation of small organic molecules with size-selected Pt<sub>n</sub> clusters supported on thin-film SiO<sub>2</sub> and MgO** — •TOBIAS HINKE, MARIAN RÖTZER, MAXIMILIAN KRAUSE, ANDREW CRAMP-TON, and UELI HEIZ — Technische Universität München, Ernst-Otto-Fischer Straße 1, D-85748 Garching bei München

To gain fundamental understanding in heterogeneous catalysis processes, model systems and associated reactions, e.g. in UHV, are useful tools. Transition metal clusters on a single crystal and metal oxide support constitute highly tunable systems. The high degree of surface uniformity of metal single crystals governs an epitaxial growth of metal oxide thin-films, forming a suitable support, which are capa-

ble of modeling bulk oxide supports. Transition metal clusters with up to 50 atoms show significant, non-scalable size-effects. Additional properties of the support, like acidity, reducibility, film thickness and interfacial support interactions, in conjunction with the crystal (local) work function affect the cluster polarization. This induces a change in surface charge density, an important quantity for metal cluster reactivity. The activity and the change of the structural sensitivity of size-selected Pt<sub>n</sub>-clusters (n=9, 10, 13) supported on SiO<sub>2</sub> and MgO thin-films are studied. Activity and structure sensitivity towards the hydrogenation of small organic molecules (ethylene and acetylene) as a model reaction are evaluated. Activity is monitored by pulsed molecular beam reactive scattering and temperature programmed desorption experiments. Characterization is performed through electronic (AES, MIES, UPS) and vibrational (IRRAS) spectroscopy.

O 85.3 Wed 18:15 P2/EG

**Photocatalytic properties of graphene-supported titania clusters calculated from *first principles*** — •SABUHI BADALOV<sup>1</sup>, RENÉ WILHELM<sup>2</sup>, and WOLF GERO SCHMIDT<sup>1</sup> — <sup>1</sup>Lehrstuhl für Theoretische Materialphysik, Universität Paderborn, 33095 Paderborn — <sup>2</sup>Institut für Organische Chemie, Technische Universität Clausthal, 38678 Clausthal-Zellerfeld

Among photocatalyst materials, titanium dioxide (TiO<sub>2</sub>; titania) draws considerable interest because of its excellent photoactivity, high oxidation potential, nontoxicity, earth abundancy, and long-standing physical and chemical stability.[1,2,3] However, its application is hampered by the lack of response to visible light and the fast recombination rate of electron-hole pairs.

In the present study, we use density-functional theory in order to explore the potential of graphene and graphene nano-flakes for photosensitizing titania clusters. It is found that the size of the graphene nano-flakes has a significant effect on the bandgap of the composite material. Besides, spatial separation of photoexcited electrons and holes is observed, which indicates prolonged lifetimes of the photoexcitation. This finding can be expected to improve the photocatalytic activity.

## References

- (1) M. Fujihira et.al., Nature 293, 206-208 (1981).
- (2) E. Wahlstrom et.al., Science 303, 511-513 (2004).
- (3) J. Schneider et.al., Chem. Rev. 114, 9919-9986 (2014).