this phenomenon has been a long-lasting enigma in the interpretation of geochemical signatures of the Earth´s mantle and the geochemistry of core-mantle differentiation. This inconsistency has been explained either by a differentiation model with a chemical equilibrium at the bottom of a silicate magma ocean while a metallic core forms at a depth of 1100 km [2] or by the so called 'late veneer' hypothesis. The later postulates an enrichment of HSE in the Earth´s mantle by an intensive meteorite bombardment 100±50 My after the Earth´s accretion [3].

So far, all the metal-silicate partitioning studies make use of 'classical' HP-HT techniques, e.g., multi-anvil press, and therefore are limited to PT conditions of the Earth´s mantle (max. 15-20 GPa/2200°C). There is urgent needs for experiments at much higher pressures and temperatures (e.g., to simulate conditions of core-mantle boundary) because it remains unclear if determined metal-silicate partition coefficients of HSE can simply be extrapolated to much higher pressures and temperatures. In the case of Pd, it has recently been shown that the partition coefficient decreases with increasing pressure (1.5 to 15 GPa) and temperature (1400 to 2200 °C) [2]. Here, we present first preliminary data on metal-silicate trace element partitioning from a new experimental approach to obtain *in-situ* information at high pressures and temperatures up to 50 GPa and 4400 K which were performed at beamline ID27 (ESRF, Grenoble, France) using double-side laser-heated diamond-anvil cells (DAC). Samples are analysed before, during and after laser heating by mean of XRF and XRD. The sample chamber was loaded with a trace element (HSE: Pd, Ru; Zr (metal incompatible)) doped chondrite glass chip placed next to a trace element free metal foil ($Fe_{90}Ni_{10}$) very close to early earth composition. Laser heating was performed at the interface of chondrite glass - metal foil and in situ XRF spectra and XRD pattern were recorded at the same time. Fluorescence analysis is used to quantify trace element concentration evolution in the melt induced by the laser heating and Diffraction patterns give information on melting stage and appearance of high pressure phases at the same time in the laser spot. First qualitative analysis verify existing data and show a strong partitioning of HSE (Pd, Ru) into the metal liquid with increasing temperature whereas Zr prefers the silicate melt. Quantitative data analyses are currently in progress.

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Structure and electronic properties of free, supported and protected clusters

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Clusters can be viewed as small representations of the crystals formed by metal. Due to finite size effects caused by their special electronic and/or ionic configurations, the properties of clusters can be substantially different from the bulk however. One example is the well known catalytic activity of small gold particles in sharp contrast to the inertness of bulk gold.

In our work, we explore the world of small metal clusters with the help of density functional theory. In particular small gold clusters are governed by strong electronic confinement effects that can be understood in a simple jellium picture. The corresponding shell closings give a unified explanation of the magic stability in ligand protect clusters [1]. This includes an alternative model for the well known Schmid "Au_{55}" cluster different from the models used in the literature. Electronic effects explain STM signatures of supported clusters and even give the possibility to determine the cluster's charge directly (see the figure) [2]. The work is extended to mixed clusters and clusters of other metals.

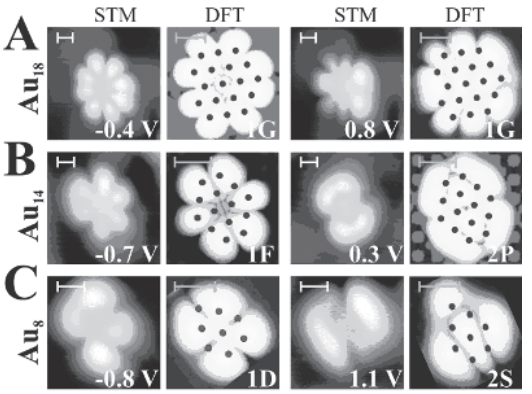

Figure: Experimental and simulated STM signatures for MgO supported gold clusters [2].

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Pushing all-electron DFT past old limits for structure of surfaces and molecules

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The prediction and our understanding of structural and chemical processes of matter benefit tremendously from the strength of today's first-principles total-energy methods. The obvious and ongoing limitations of these methods are:

- the affordability and accuracy of the physical approximations [in density functional theory (DFT), primarily the exchange-correlation functional]
- but in addition, the affordability and accuracy of all other numerical approximations that lead to a total energy for a given structure.

For few-atom structures, serial structure screening, exhaustive structure predictions and meaningful time scales in molecular dynamics are now routinely possible, but the challenge still grows immensely for larger system sizes. The present work describes some recent efforts to push out these limits further, using all-electron density functional theory as implemented in the numeric atom-centered orbital based code package FHI-aims [1]. We show how accurately the classic large-scale surface reconstruction of Au(100) and Pt(100) are captured in terms of structure and energetics by current all-electron DFT - *if* large enough structure approximants (up to ~1000 atoms in a slab model) are considered [2]. We then comment on the additional challenges encountered for the structure and dynamics of biochemical molecules at the other end of the periodic table, addressing both the structure and high-temperature stability of a series of polyalanine-based peptide molecules (up to 180 atoms) in the gas phase. In particular, we find that van der Waals interactions are of unexpectedly large relevance to stabilize specifically the "classic" α-helical structure over competing conformations (even in the gas phase) [3]. Our results are directly verified by comparing theoretical infrared spectra from basis-set