Work Plan for the CSIC visit in Madrid

Recently, Martin Schnedlitz and Ralf Meyer, two PhD students in the Hauser group, have developed a “hybrid” potential from two sources in order to improve the description of metallic interactions in Ni- and Au-containing nanostructures. By now, several structural predictions have been made already for smaller mixed-metallic clusters, which are in good agreement with our recent experimental findings obtained via transition electron microscopy of He-droplet grown core@shell Ni@Au nanoparticles. However, the actual dynamics observed by *in situ* heating are not fully understood yet.

It is the aim of this STSM to embed Martin Schnedlitz in ongoing research activities in the group of Dr. María Pilar de Lara-Castells, using their expertise to perform large-scale atomistic molecular dynamics simulations on the NiAu system. The planned work can be split into two smaller packages; each of them should take approximately a week to set up; of course, larger computations, in particular those in the context of dynamics simulation, will take much longer than the proposed stay, but are supposed to be planned efficiently and then suitably distributed among the available computer facilities in Madrid and Graz.

WP1: The first part is dedicated to the investigation and visualization of crystal structure tension depending on particle size and composition, preferably evaluated for different interatomic potentials, to learn about specific features and capabilities of various approximations. Hopefully, this static modelling by itself will reveal already certain insights into why de-centralized Ni core positions are energetically more preferred than fully centralized arrangements.

WP2: The second part will be focusing on molecular dynamics simulations, attempting to model diffusion processes at higher temperatures in order to understand the impact of high surface-to-volume ratios on shape and structure of thermodynamic phase diagrams. Phenomenologically motivated “corrections” of bulk phase diagrams should be compared to results obtained in the atomistic picture using a suitable interaction potential.