

Adsorption of element 112 on Au surface

C. Sarpe-Tudoran¹, J. Anton¹, W. Sepp¹, B. Fricke¹, V. Pershina²

¹ Universitat Kassel, Germany

² GSI, Germany

ctudoran@physik.uni-kassel.de

The adsorption of element 112 on a gold surface is studied using the full relativistic four-component ab initio density functional (DFT) cluster calculations. The binding energy and bond length is determined, as well the adsorption position relative to the surface atoms sites. The use of optimized numerical atomic wave functions in the MO-LCAO procedure in the DFT method offers a flexible basis for the expansion of the MO orbitals. Because the adsorption phenomenon is dominantly local, we use clusters of different sizes to approximate the surface. In addition we apply the embedded cluster method. This procedure uses an inner part of 22 and 28 atoms (depending of the symmetry of the adsorbate-cluster surface) which is made self consistently. The surrounding atoms which account for the environmental influences to the inner cluster, is divided in two parts (transition environment and external environment) which are treated in different ways in the description of the interaction with the inner part. Finally potential energy curves and diagrams for the density of states for the system under consideration are presented. The results from size convergent cluster calculations are compared with the results of the embedding calculations.