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Adsorption behavior of super-heavy elements (Z ≥ 112) on metal and inert surfaces

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Investigation of chemical and physical properties of the heaviest elements (those beyond Lr) is a hot topic since several decades. In this time period, many new elements were discovered and after a proper characterization were added to the Periodic Table of the elements. The main problem of such investigations, however, is the rather short half-life of these elements, which requires the development of innovative experimental techniques. Nowadays the research focusses on the chemical properties of the element 114. So far, two gas chromatography experiments to study the interaction strength of element 114 with a gold surface have been performed with conflicting results. One experiment [1] reported a weak interaction of element 114 with a gold surface, leading to adsorption only at very low temperatures of approximately -90°C, while in the second experiment [2] adsorption on gold has been observed at the room temperature, indicating a much stronger bond between element 114 and gold. To resolve this conflict, further experiments on chemical properties of the element 114 will be performed at GSI and PSI/JINR in the next two years. For theoretical studies, standard quantum-mechanical packages that treat a system mostly non- or only scalar-relativistically are not satisfactory: Due to rather significant relativistic effects on the electron shells of the heaviest elements a fully-relativistic four-component description is required.
Recently, we have studied the adsorption behavior of elements 112, Cn, and 114 and their lighter homologues Hg and Pb, respectively, on gold surfaces [3] by using a cluster-approach [4]. We found that Hg/Cn and Pb/114 prefer different adsorption sites. Also, the adsorption energies of elements 112 and 114 are related to those of their lighter homologues in a different way. Thus, Eb(Cn) is only slightly (0.1-0.2 eV) lower than Eb(Hg), while Eb(114) is much lower (1.4 eV) than Eb(Pb). This is due to the fact, that in element 112 both the relativistically stabilized 7s and destabilized 6d AOs take part in the binding, while for element 114 binding is mostly determined by the relativistically stabilized 7p1/2 orbital. In contrast to Pb, where 6p3/2 strongly contributes to the surface bond, the 7p3/2 participate much less due to its large relativistic destabilization (the spin-orbit splitting between 7p1/2 and 7p372 is about 3.5 eV). Furthermore, binding of element 114 to gold is similar to that of Cn, however, about 0.2 eV stronger. Our predicted sequence in the Eb values is Cn < Hg < E114 « Pb. Thus, we predicted that in the thermochromatography experiments, element 114 will adsorb right at the beginning of the chromatography column with the hot end of 35°C, at the position of Hg. This prediction was recently confirmed experimentally [2].
In this talk we will present theoretical results on adsorption energies and distances of the elements from 112 to 114 and their homologues on metal (gold) and inert (SiO2) surfaces.

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References

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Primary author: Dr ANTON, Josef (University of Ulm)

Presenter: Dr ANTON, Josef (University of Ulm)

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