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Adsorption of the nihonium species on gold surface: a relativistic density functional theory study

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The discovery of long-lived isotopes of superheavy elements (SHEs) in nuclear fusion reactions of ^{48}Ca with actinide targets signifies a close approach to the island of particularly shell-stabilized nuclei. While the emergence of the new elements is a fantastic discovery itself, the longevity of certain isotopes is thought-provoking for chemical investigations, both experimental and theoretical. Successful chemical identification of copernicium (element 112, Cn) and flerovium (element 114, Fl) has been recently followed by the recognition of the discovery of nihonium (element 113, Nh) confirmed at the fourth IUPAC/IUPAP Joint Working Party. Although preliminary experimental results have been recently obtained in FLNR JINR (Dubna), the chemical properties of nihonium remain of top interest. From the theoretical standpoint, investigations of the SHE chemistry are especially challenging as they require an understanding of the electronic structure in the presence of strong fields of heavy nuclei and thus governed by relativistic effects.

Gas thermochromatography on gold is a unique method of chemical detection of SHEs. The corresponding experiments, however, are extremely sophisticated and expensive and produce very scarce data on the chemical properties of SHEs. Moreover, the correct and detailed interpretation of the available experimental data cannot be performed without preliminary theoretical modeling. The main effort of our research is focused on the description of the SHEs atoms/molecules adsorption on a gold surface from first principles – a key component for quantitative theoretical predictions. The desorption energies of SHEs on a gold surface are estimated using the cluster model. To simulate the electronic structure of such systems, we combine accurate shape-consistent relativistic pseudopotentials and non-collinear two-component relativistic density functional theory. As an important result of such modeling, we recommend estimates of the Nh desorption energies on gold – 110 kJ/mol.

Strong relativistic effects suggest dramatic dissimilarities in the chemical behavior of SHEs and their formal lighter homologues. The calculated adsorption energy for single atoms of nihonium on a gold surface differs substantially from the experimentally measured adsorption energy on gold of its nearest homolog, thallium. This casts doubt on the usefulness of the experiments with Nh formal homologues for understanding its chemistry. Despite manifest deviations of the chemical properties of the SHEs from the trends observed in their lighter formal homologues in the respective groups of the periodic table, finding chemical pseudo-homologues appears a practically meaningful issue.

It has been shown experimentally that the desorption temperatures and energies of Cn and Fl atoms from a gold surface are fairly close to each other and overall lower than those of their immediate homologs Hg and Pb, observed on the same surface. This confirms theoretical predictions concerning the electronic structure of Cn and Fl atoms: the strong relativistic stabilization of the s and p_{1/2} shells in both Cn ($6d^{10}7s^2$) and Fl ($6d^{10}7s^27p_{1/2}^2$) results in a closed-shell character of the ground states of these atoms. Due to this unique feature of the 7th row of the Periodic Table, the electronic structure of a Nh atom can be interpreted as a Fl atom with a hole in its closed $7p_{1/2}$ subshell. This observation seems to render astatine a closer chemical “relative” of Nh in comparison to the formal homologue Tl. Thus, At might be a plausible chemical species for model experiments aiming at finding the optimum experimental conditions for further explorations of the Nh chemistry. The predicted adsorption energies for At and AtOH on gold are 130 ± 10 kJ/mol and 90 ± 10 kJ/mol, respectively. This confirms the experimental observation on the formation of AtOH molecules in presence of trace amounts of water and oxygen in the carrier gas. Due to the similarities in the chemical properties of

AtOH and NhOH molecules, one may expect, that the formation of NhOH is indeed possible under experimental conditions similar to those in the experiments on At.

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