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First-principles theoretical study of adsorption properties of heavy and superheavy elements and their compounds on selected surfaces

ABSTRACT

Gold and Quartz are materials coating detectors that are used in the preparation of superheavy elements in so-called atom-at-a-time experiments. Within them, synthesized atoms and their possibly formed molecules adsorb onto the surface, and experimentalists estimate their adsorption enthalpy. In my online talk, I give a review of several first-principles theoretical studies on the adsorption properties of heavy and superheavy elements and their compounds on the above-mentioned surfaces. Such predicted results provide assistance to experimentalists concerning the identification of adsorbed species. The main computational apparatus was the relativistic periodic DFT, as implemented within the AMS BAND program suite. To name a few of our studies, in [1], we investigated the adsorption properties of group 1 and 2 elements Cs, Fr, E119, Ba, Sr, and E120, as well as group 1 hydrides and hydroxides on hydroxylated quartz surfaces. In [2], adsorption energies, E_{ads}, of a superheavy element (SHE), Lv, and its lighter homologue, Po, as well as those of their oxides, hydrides, and hydroxides, on hydroxylated quartz surfacesare calculated. It was shown that elemental Po and Lv should be the most volatile out of all the considered species over the quartz surface, with Eads on the order of van der Waals bond energies. Likewise, in [3], E_{ads} of oxides and oxyhydrides of the superheavy element Ts and its lighter homologue At on the gold surface are predicted and discussed.

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[2] V.Pershina, M.Iliaš, Mol.Phys., 2025, https://doi.org/10.1080/00268976.2025.2573831
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BIOGRAPHY

Miroslav Iliaš (https://orcid.org/0000-0002-8038-6489) finished his PhD. studies at Comenius University Bratislava in 2002. He is working in the field of Theoretical and Computational Chemistry. His research interests are applications of computational chemistry methods for assisting experiments of superheavy elements synthesis