



Adsorption of superheavy element atoms and molecules on different surfaces

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The present work is a continuation of our research on adsorption of superheavy elements (SHEs) on surfaces of detectors of a chromatography column used in gas-phase experiments.¹ This time, adsorption energies, E_{ads} , and other properties of atoms and oxides of Cn and Fl, as well as of homologous species of Hg and Pb, on the Au(111) and hydroxylated quartz surfaces are predicted on the basis of 2c-DFT calculations and a periodic slab model using the BAND software. The ambition of the work is to interpret the outcome of the “one-atom-at-a-time” gas-phase chromatography experiments on reactivity/volatility of Fl.² A significant difference in the adsorption strength was found between the elements and their oxides. Also, geometries of the adsorbed MO species were shown to be very different between group 12 and 14.

Some new aspects for adsorption of group 13 elements, Tl and Nh, on hydroxylated quartz surfaces are discussed.

References

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- [2] A. Yakushev, et al., *Chem. Phys. Chem.*, submitted