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Superheavy Element Chemistry Through Highly Accurate Small-Core Pseudopotential Model

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Recent advances in first-principle based studies of superheavy element (SHE) chemistry using the new accurate small-core pseudopotential model are summarized. This model accounts for the finite nuclear size and effectively incorporates most relativistic effects described by the all-electron Dirac—Coulomb—Breit model (including the bulk of Breit interactions) and enables explicit correlation of both valence and subvalence electrons. It provides thus a good basis for attaining optimal accuracy/cost ratio in the cases of large and strongly interfering relativistic and correlation effects characteristic for the SHE compounds. Depending on the size of systems under study and required accuracy, high-level relativistic wavefunction theory (mainly coupled-cluster) and density functional theory methods or their combinations were used to solve the electron correlation problem.

Synthesis and chemical identification of new superheavy elements is of top interest during the last decade. Since the thermochromatography on gold has been proved to be a unique method of chemical detection of heaviest elements, main attention was paid to the description of the SHEs – gold interactions. Adsorption energies of SHEs on gold surface were estimated using the cluster model. Its reliability was improved by monitoring charge distributions in the vicinity of the adsorption site and taking into account the effects of relaxation of the cluster compatible with its embedding into the crystal. In some cases the results differ significantly from those of previous theoretical studies. For instance, the new estimates of element 113 and element 120 on gold adsorption energies (1.0-1.2 eV and 2.5-2.7 eV respectively [1, 2]) are recommended.

Further development of the SHE "chemical" identification techniques may benefit from having a broader view of their chemical properties. We performed systematical relativistic calculations of molecular structures and energetics of presumably stable binary compounds of SHEs with the most common light elements. We focus on the properties of element 120, copernicium (E112) and flerovium (E114) which are expected to display particularly strong relativistic contraction and stabilization of the filled s or p1/2 subshells. The obtained results along with the similar data for the homologues of SHEs were visualized through the "chemical graphs" which reflect the main trends in changing basic gas-phase chemical properties of the elements in the given group of the Periodic table and demonstrate the specificity of SHEs [3].

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