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Relativistic Quantum Chemistry for Chemical Identification of the Superheavy Elements

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One of the main aims of studies in the area of the chemistry of the heaviest elements is to place a newly produced element in the proper position of the Periodic Table [1]. It is achieved by comparing behaviour of the new element with that of its lighter homologs in the chemical group. Having this in mind, a large number of interesting and important chemical experiments on the heaviest elements were performed in the recent years [2]. Theoretical investigations in this area have also been very fruitful and resulted in some remarkable achievements [2,3]. In the presentation, recent advances in the relativistic electronic structure calculations for the heaviest elements and predictions of their experimental behaviour are overviewed.

For the heaviest elements, electronic structure calculations should be made with the use of methods that treat relativistic and electron correlation effects at the highest possible level of theory. In the recent years, the relativistic quantum theory and computational algorithms received tremendous developments [4]. As a result, very accurate calculations of the electronic structure and properties of superheavy atoms and molecules became possible. On their basis, reliable predictions of experimental behaviour of these elements in the sophisticated and expensive experiments with single species have been made [5].

For atoms, Dirac-Coulomb-Breit (DCB) calculations with electron correlation at the highest level of theory, i.e., a coupled-cluster (CC) method, were performed for elements till Z=122 [6]. In the molecular theory, fully relativistic (4-component) and 2-component wave-function (*ab initio* Dirac-Fock) [7] and Density-Functional-Theory (DFT) [8] methods have been developed to such an extent that very accurate predictions of binding molecular energies, optimized geometry, electronic density distributions, etc. are now available. On their basis, predictions of experimental behaviour of elements Rf through Hs and of Cn and Fl for gas-phase and aqueous chemistry chromatography experiments have been made [2,3,5]. Interesting cases of volatility of even heavier elements, like 115, or 119 and 120 are considered [9].

Influence of relativistic effects on properties and experimental behaviour of the heaviest elements is elucidated. Future perspectives for the chemical studies on the heaviest elements from the theoretical point of view are outlined.

＊ The talk will be given in English language..

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