



Electronic structure and properties of superheavy elements

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Received 29 December 2014; received in revised form 15 April 2015; accepted 19 April 2015

Available online 23 April 2015

Abstract

Spectacular developments in the relativistic quantum theory and computational algorithms in the last few decades allowed for accurate calculations of properties of the superheavy elements (SHE) and their compounds. Often conducted in a close link to the experimental research, these investigations helped predict and interpret an outcome of sophisticated and expensive experiments with single atoms. Most of the works, particularly those related to the experimental studies, are overviewed in this publication. The role of relativistic effects being of paramount importance for the heaviest elements is elucidated.

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Keywords: Superheavy elements; Electronic structure; Properties; Relativistic effects

1. Introduction

At the modern level of the relativistic quantum theory, atomic electronic ground states, needed for placement of the new elements in the Periodic Table, can accurately be predicted till $Z = 122$ (see the chapter of Eliav et al., in this issue). Nevertheless, studies of chemical properties, both theoretical and experimental, are extremely important: they try to find an analogy in the chemical behaviour of the heaviest elements with that of the lighter homologs in the chemical groups in order to justify their position in the Periodic Table defined by Z and by the electronic ground

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state [1–3]. It is meanwhile well recognized that relativistic effects on the electron shells of the superheavy elements (SHE) strongly influence their properties [4–9].

Experimentally, useful information is obtained from the state of the art “one-atom-at-a-time” chemical experiments [1–3]. They are based on the principle of chromatographic separation either in the gas phase exploiting differences in volatility of SHE atoms or their compounds [10,11], or in the aqueous phase assessing differences in the complex formation [12]. Such chemical studies are performed with SHE isotopes having a sufficiently long life-time for the chromatography separation processes [13], even though all the transactinide elements from $Z = 104$ through $Z = 118$ are presently known [14]. Consequently, fast gas-phase experiments were performed for elements Rf through Hs, Cn and Fl, whose isotopes have half-life, $t_{1/2}$, of the order of at least one second [3,10,11], while aqueous chemistry experiments, that are more time-consuming, mainly because of the time needed for the preparation of a sample suitable for α -spectroscopy, require isotopes with longer $t_{1/2}$ (of the order of minutes). Therefore, only the complex formation of Rf, Db, and Sg has so far been investigated [12].

The chemical experiments are, however, restricted to the measurements of volatility, complex formation and redox potentials (in few cases) only. Knowledge of many other properties important for placement of the new elements in the Periodic Table, or establishing an analogy with the lighter congeners cannot be presently experimentally accessed at all. This knowledge includes stability of species (also of oxidation states), geometrical configurations, ionization potentials (IP), electron affinities (EA), type of bonding, etc. Even the chemical composition of the studied compounds is, as a rule, unknown. It can only be assumed by analogy in the behaviour of the heaviest elements with that of their lighter homologs studied under the same conditions. Thus, in this part of the Periodic Table theory plays an extremely important role and is often the only source of useful chemical information. It is also invaluable in predicting and/or interpreting an outcome of the sophisticated and expensive experiments with single atoms. Moreover, it is the theory that can reveal how relativistic effects influence chemical properties: only by comparing the behaviour observed experimentally with that predicted on the basis of relativistic vs. non-relativistic calculations, can the importance and magnitude of relativistic effects be established.

There is quite a number of reviews on quantum-chemical calculations of properties of SHE [2–9]. The most comprehensive issues on the physics, chemistry – both experiment and theory – of the heaviest elements are those of [1–3]. General aspect of the chemistry of the SHE based on theoretical arguments has also been discussed earlier by Seaborg and Keller [15,16]. The present publication is a short overview of the recent achievements in his area. A special attention is drawn to the works related to the experimental studies.

2. Quantum-chemical methods and approaches

It is known that starting from the 6th row of the Periodic Table relativistic effects cannot anymore be neglected: they are responsible for quantitative and qualitative changes in properties [17]. For elements with $Z = 104$ and higher, they are even more important [4–9], so that the usage of relativistic methods for this part of the Periodic Table is indispensable. For reliable predictions, the methods should treat relativistic and correlation effects at the highest possible level of theory, because both types of the effects contribute significantly to the bond strength and other properties of SHE systems. Some special approaches that bridge calculations with quantities that cannot be presently predicted from the calculations are also useful.

Most of the modern relativistic electronic structure methods are described in [18–24]. Atomic codes and their application to SHE are overviewed in the chapter of Eliav et al. in this issue, as

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