FIRST PRINCIPLE BASED MODELING AND INTERPRETATION OF CHEMICAL EXPERIMENTS ON SUPERHEAVY ELEMENT IDENTIFICATION*

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Abstract. *Our latest advances in studies of actinide and superheavy element (SHE) chemistry using the shape-consistent two-component small-core relativistic pseudopotential (RPP) method and two-component relativistic density functional theory (2c–RDFT) are summarized. The features of these elements, due to large relativistic effects, are emphasized. The RPP model, leaving for explicit correlation treatment with both valence and subvalence (outercore) electrons, accounts for the finite nuclear size and incorporates relativistic effects (including the bulk of Breit interactions), providing a good basis for attaining optimal accuracy/cost ratio in the cases of large and strongly interfering relativistic and correlation effects, intrinsic for the heavy-atom compounds. The RPP/2c–RDFT approach allows one to solve the outercore-valence many-electron problem with moderate computational expenses while using practically exhaustive basis sets, optimized for the case of large differences between nl(j=l+1/2) and nl(j=l-1/2) one-electron states. Because of the exceptional role of thermochromatography on gold in the experiments on the "chemical" identification of SHEs with atomic numbers Z ≥ 112, the main attention was paid to the description of the SHE – gold interactions. Adsorption energies of SHEs on a gold surface were estimated using the cluster model. Its reliability was improved by monitoring the charge distributions in the vicinity of the adsorption site, taking account of the effects of the relaxation of the cluster compatible with its embedding into the crystal. The resulting desorption energy estimates for elements 113 and 120 single atoms from gold surface are substantially lower than the previously reported values.*

Key words: *Relativistic pseudopotential, relativistic effective core potential, relativistic density functional theory, actinides, superheavy elements, correlation effects*

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1. INTRODUCTION

First principle based electronic structure modeling for molecules or clusters containing superheavy element (SHE) atoms require, in general, accounting for relativistic effects on equal footing with the electronic correlation. The straightforward way to do so is to solve the electron correlation problem for the Dirac–Coulomb(–Breit) relativistic Hamiltonian, implying the use of the four-component wave functions. However, such a way dramatically increases the computational cost compared to the corresponding nonrelativistic calculations that is particularly tedious in simulation of adsorption of a superheavy element on a surface. A most attractive alternative is to use relativistic pseudopotential (RPP) or Relativistic Effective Core Potential (RECP) theory (RPP below) since modern formulations of the theory are pretty accurate and economical. Another advantage of RPP is its good compatibility with well-developed nonrelativistic DFT versions in contrast to the all-electron relativistic DFT formulations. Below we discuss some theoretical and computational features of RPP practice for such objects.

2. RELATIVISTIC PSEUDOPOTENTIAL METHOD

The RPP method is most widely used in calculations on molecules and clusters containing heavy atoms because it drastically reduces the computational cost at the integral generation, self-consistency and integral transformation stages. When core electrons of a heavy-atom molecule do not play an active role, the effective Hamiltonian with RPP can be presented in the form

$$H^{Ef} = \sum_{i_v} [h^{Schr}(i_v) + U^{Ef}(i_v)] + \sum_{i_v, j_v} \frac{1}{r_{i_v j_v}}. \quad (1)$$

The Hamiltonian in Eq. (1) is written only for a valence subspace of electrons, which are treated explicitly and denoted by indices i_v and j_v (the large core approximation). As in the case of non-relativistic pseudopotentials (PP), this subspace is often extended by inclusion of some outermost core shells for better accuracy (the small core approximation) but below we consider them as the valence shells because these outermost core and valence shells are not treated here using different

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approximations. In Eq. (1), h^{Schr} is the one-electron Schrödinger Hamiltonian

$$h^{Schr} = \frac{-1}{2}\nabla^2 - \frac{Z_{ic}}{r}, \qquad (2)$$

where Z_{ic} is the charge of the nucleus decreased by the number of inner core electrons. U^{Ef} in Eq. (1) is an RPP operator that is usually written in the radially-local (semi-local) approximation [1,2,3] when the valence pseudospinors are smoothed in heavy-atom cores. Among the radially-local RPPs, the shape-consistent (or norm-conserving) RPP approaches [4] are most widely employed in calculations of heavy-atom molecules, though "energy-consistent" RPPs by Stuttgart-Dresden team are also actively used [5]. In plane-wave calculations of solids and in molecular dynamics, the separable PPs [6] are more popular now because they provide linear scaling of computational effort with the basis set size for self-consistent-field-like procedures in a more straightforward way than the radially-local PPs. Moreover, the nonlocal Huzinaga-type "*ab initio* model potentials" [7] conserving the nodal structure for the valence spinors are often applied. Contrary to the four-component wave function used in Dirac-Coulomb(-Breit) (DC(B)) calculations, the pseudo-wave function in the RPP case can be both two- and one-component. The PP operator simulates, in particular, interactions of the explicitly treated electrons with those, which are excluded from the PP calculations. The use of the effective Hamiltonian in Eq. (1), instead of all-electron four-component Hamiltonians, raises the issue about its accuracy. It was shown both theoretically and in calculations [8,9,10] that a typical accuracy of the radially-local RPPs is within 1000-3000 cm^{-1} for transition energies between low-lying states.

In our papers [9,11,12], the conventional radially-local (semi-local) form of the RPP operator (used by many groups up to now but suggested and first applied about 50 years ago [1,2,3]) was shown to be limited in accuracy, and some nonlocal corrections to the RPP operator were suggested [11,12,13,14], which have allowed us to improve significantly the RPP accuracy [8,9,10,12]. Moreover, it is known that the Breit interaction can give contributions in excess of one thousand wave numbers even to energies of transitions between lowest lying states of very heavy elements [15,16]. It is also clear that the point nuclear model becomes less appropriate when the nuclear charge is increased. Therefore, the RPPs designed for accurate calculations of actinide and superheavy element (SHE) compounds should allow one to take into account the Breit interaction and the finite size of nuclei. The most economic way is to incorporate the corresponding contributions into the RPP operator.

In a series of papers (see Refs. in [17]), a Generalized RECP (GRECP) approach was developed, that involves both radially-local, separable and Huzinaga-type potentials as its components in particular cases. Additionally, the GRECP operator can include terms of other types, known as "self-consistent" and two-electron "term-splitting" corrections [14], which are important particularly for economical (but precise) treatment of transition metals, lanthanides and actinides. With these terms, the accuracy provided by GRECPs can be even higher than the accuracy of the "frozen core" approximation (employing the same number of explicitly treated electrons) because they can account for relaxation of explicitly excluded (inner core) electrons. In contrast to other RECP methods, GRECP employs the idea of separating the space around a heavy atom into three regions: inner core, outer core and valence, which are first treated employing different approximations for each. The outer core pseudospinors (nodeless) together with valence pseudospinors (nodal) are used for constructing the GRECP components [18]. Quantum electrodynamics effects (QED) (see [15,16]), arbitrary nuclear models, and correlation with inner core shells [19] can be efficiently treated within GRECP. It allows one to attain practically any desired accuracy for compounds of lanthanides, actinides, and SHEs as well, while requiring moderate computational efforts since the overall accuracy is limited in practice by possibilities of correlation methods.

3. RPP ACCURACY: EXAMPLE OF CORRELATION CALCULATIONS OF THE E120 ATOM

Main difficulties of quantitative electronic structure modeling for SHE-containing compounds arise from huge amplitudes of relativistic effects, which have no analogues in compounds of elements from the remaining part of the Periodic table. From the computational point of view, the critical issue is the high intensity of magnetic interactions reducing the symmetry of the many-electron problem and thus leading to a dramatic increase in the amount of required calculations in comparison with similar non-relativistic or scalar relativistic problem (where magnetic interactions switched off). Moreover, the neglect of these interactions is unacceptable even for constructing reasonable zero-order approximations for subsequent perturbative treatment of the electronic states under study. Furthermore, relativistic contraction of low-angular-momentum shells (s, $p_{1/2}$) along with the secondary expansion of those with high angular momenta (d and f) leads to a strong overlapping of radial distributions of shells with different principal quantum numbers, so-called blurring of the shell structure (see Fig. 1).

It is therefore difficult to separate a small subset of electronic shells, which can be exempt from the correlation treatment without loss of accuracy of the calculated characteristics of low-energy processes; normally the number of electrons which should be correlated turns out to be unexpectedly large. Finally, the correlations and magnetic interactions strongly interfere and their independent description is senseless. In this situation the use of highly accurate ab initio techniques of the wave function theory is extremely expensive and thus restricted to small systems; relativistic density functional theories (RDFT) seem to provide an attractive alternative with acceptable reliability/cost ratio.

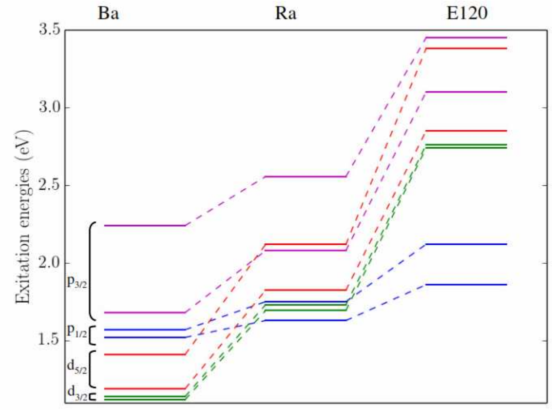

Figure 1. Comparison of the lowest $ns^2 \rightarrow nsnp_j$, $ns(n\text{-}1)d_j$ excitation energies (eV) for Ba (n=6), Ra (n=6) and E120 (n=8) atoms [20, 23].

Let us compare GRECP [20] and relativistic energy consistent pseudopotential (RECPP) [21] on the example of the E120 atom, for which the results of both all-electron DCB and RPP calculations on the excitation energies were recently published by different authors [20,21,22,23,24]. The contributions from both Breit interactions and the finite nuclear size were taken into account in the above calculations. Moreover, the calculations [21,23] take into account other QED effects (the various Lamb-shift terms, i.e. the self-energy and vacuum polarization), but their contribution in the excitation energies for E120 is about 100 cm^{-1} (see tables IV in [21] and VII in [23]), therefore the QED effects can be neglected compared to the level “chemical accuracy” (about 1 kcal/mol or 350 cm^{-1}) and the level of accuracy of accounting for the correlation effects in the vast majority of modern molecular calculations. It should be noted that the number of electrons explicitly treated in RPP calculations is 10 for GRECP ($7s^27p^68s^2$) and 28 for the RECPP ($6s^26p^66d^{10}7s^27p^68s^2$). (Obviously, the computational costs of the calculations increase rapidly with the number of explicitly treated electrons.) Due to the absence of any experimental data for E120, (this SHE has not yet been synthesized, although attempts to obtain E120 are underway [25,26]), the only way to reliably estimate the RPP accuracy is a comparison of the results of all-electron calculation with DCB Hamiltonian (and, of course, with accounting for the finite nuclear size) and calculation with the corresponding RPP. The required all-electron calculations of the excitation energies of the E120 atom carried out by different authors are presented in Table 1. The correlation effects were taken into account by the combined method of many-body perturbation theory, linearized coupled clusters with single and double cluster amplitudes, and configuration interaction (MBPT/LCC-SD/CI) in paper [23], by relativistic coupled-cluster method in Fock space with single and double cluster amplitudes (RCC-SD) [20], and by relativistic coupled-cluster method in Fock space within the extrapolated intermediate Hamiltonian approach (RCC-IH) [21,24]. It should be mentioned that the different numbers of electrons were correlated in these calculations, see the second line in the heading of Tables 1 and 2. One can see from Table 1 that the results of the three calculations in the 3-5 columns are in good mutual agreement (provided that the quite different methods were used to account for the correlations and so on), whereas the results from the sixth column [21] are significantly different (another order of the atomic levels is even predicted). One can see from the third column of Table 2 that accounting for the correlations of only 10 electrons is already sufficient for attaining the “chemical accuracy”. Moreover, the GRECP method (the fourth column) allows one to reproduce the all-electron results with high accuracy (the GRECP errors are comparable with the small variations in the three first well-matched all-electron results in Table 1). The RCC-IH results [21] are again strongly deviated.

Table 1. Excitation energies for the E120 atom obtained by different authors in all-electron correlation calculations (in cm^{-1})

Leading relat. config	Relat. term	DC(B) MBPT /LCC-SD/CI [23]	DCB 52e-RCC-IH [24]	DCB 28e-RCC-SD [20]	DCB 28e-RCC-IH [21]
$8s_{1/2}^2$	(J=0)	→			
$8s_{1/2}^1 8p_{1/2}^1$	(J=0)	15936	15648	15328	20820
$8s_{1/2}^1 8p_{1/2}^1$	(J=1)	17920	17587	17382	23124
$8s_{1/2}^1 7d_{3/2}^1$	(J=1)	22865	22903	22337	32026
$8s_{1/2}^1 7d_{3/2}^1$	(J=2)	23283	23034	22494	32065
$8s_{1/2}^1 7d_{5/2}^1$	(J=3)	23813	23782	23377	32165
$8s_{1/2}^1 8p_{3/2}^1$	(J=2)	25651	25192	25308	29254
$8s_{1/2}^1 7d_{5/2}^1$	(J=2)	27477	27247	27652	37529
$8s_{1/2}^1 8p_{3/2}^1$	(J=1)	27669	27513	28304	33301
$8s_{1/2}^1$	(J=1/2)	47682	47089	47633	47358

Table 2. Excitation energies for the E120 atom obtained from equivalent all-electron and RPP correlation calculations (in cm^{-1})

Leading relat. config	Relat. term	DCB 10e-RCC-SD [20]	GRECP 10e-RCC-SD [20]	DCB 28e-RCC-IH [21]	RECPP 28e-RCC-IH [21]
$8s_{1/2}^2$	(J=0)	→			
$8s_{1/2}^1 8p_{1/2}^1$	(J=0)	15012	15278	20820	20792
$8s_{1/2}^1 8p_{1/2}^1$	(J=1)	17064	17315	23124	23101
$8s_{1/2}^1 7d_{3/2}^1$	(J=1)	22207	22573	32026	32035
$8s_{1/2}^1 7d_{3/2}^1$	(J=2)	22259	22646	32065	32036
$8s_{1/2}^1 7d_{5/2}^1$	(J=3)	22968	23354	32165	32199
$8s_{1/2}^1 8p_{3/2}^1$	(J=2)	25009	25262	29254	29245
$8s_{1/2}^1 7d_{5/2}^1$	(J=2)	27271	27615	37529	37511
$8s_{1/2}^1 8p_{3/2}^1$	(J=1)	27834	28141	33301	33320
$8s_{1/2}^1$	(J=1/2)	47120	47453	47358	47371

3. MODELING OF ADSORPTION COMPLEXES OF SUPERHEAVY ELEMENT ATOMS ON GOLD SURFACE

Ab initio approaches can be used to systematically improve the estimates of physical parameters, approaching the precise solution for the selected Hamiltonian model. This fact is particularly important for the prediction of properties of SHE compounds. Thus, it becomes possible to control the reliability of the results in the absence of experimental data. High-precision *ab initio* relativistic calculations require large computing resources, which sharply limits the field of their application. The RDFT is an efficient tool for calculating properties of systems comprising ~10^2 heavy atoms, which is, in particular, sufficient for the estimation of the principal adsorption characteristics of SHEs on different surfaces (including the surfaces of heavy transition metals) using the cluster model.

The central practical problem of any Kohn-Sham-like formulation is the appropriate choice of approximate exchange-correlation functional (XCF). The non-relativistic form of kinetic energy and electron-electron repulsion operators in RPP Hamiltonian would justify the straightforward use of conventional non-relativistic XCFs in the frames of the RDFT. However, there are at least two stumbling blocks on this way. First, the non-relativistic XCFs normally depend on both charge and spin density, but the latter entity fully loses its invariant sense for systems with strong spin-orbit interactions. Theoretically, relativistic energy should be a functional of charge density and three components of vector magnetization density; in practice, the dependence on the three components is replaced by that on the absolute value of spin part of the magnetization density (non-collinear approximation). Second, although DFT is commonly classified as *the first principles* based approach, the construction of most popular approximations for the exchange-correlation functional took into account experimental (mainly thermodynamical) data on light element compounds. Therefore their use in the studies of SHE chemistry is a pure (and therefore dangerous) extrapolation.

The data on SHE compounds required for the exchange-correlation functional calibration can be obtained from highly accurate ab initio calculations. Since fully relativistic high-level correlation methods are practically applicable only to very small molecules and while reliable calibration requires the information of rather complex systems, the most straightforward way to get the input data consists in using combined ab initio / RDFT schemes [27]. The potential energy of the electronic ground state of the system as a function of geometric parameters of the molecule or the cluster, which are evaluated by high-precision *ab initio* calculations with the scalar part of the Hamiltonian (1), is corrected for magnetic (effective spin-orbit) interactions. This correction, which also depends on the geometric parameters, is estimated by comparing the results obtained by RDFT with the total and scalar Hamiltonians. It is essential that the corrections depend on the particular approximation for the XCF to a much lesser extent than the binding energies. The combined scheme provided the most reliable data on interactions of the element 112 (Cn) and element 113 (E113) atoms with small (up to 4 atoms) gold clusters [28, 29]. These cluster sizes are obviously insufficient to reliably evaluate the adsorption energy on gold surface in the frames of the combined scheme. Such estimations are very popular among experimentalists, since the thermochromatography on gold has been proved to be a unique method of chemical detection of heaviest elements. The adsorption of single atoms of elements 112 (copernicum, Cn) and 114 (flerovium, Fl) on a gold surface has been recently studied by this technique [30, 31]. The desorption energy values derived from the results of these experiments are 0.54 eV for Cn and 0.39 eV for Fl. According to fully relativistic (four-component) DFT calculations of Cn and Fl single atoms with gold systems, from an atom to an Au_n cluster simulating the Au (111) surface, Fl should be more reactive than Cn [32]. Article [28] deals with the problem of finding the origin of this disagreement between the RDFT results and the estimations based on experimental data for Cn and its lighter homolog, Hg, atoms on gold surface. In this area further efforts are needed.

Nowadays, investigation of element 113 (E113) chemical properties is of top interest, and the first thermochromatographic experiment in this area has already been carried out [33]. Adsorption of E113 and E120 single atoms on the stable Au (111) surface was studied in the framework of the cluster model [34, 35]. We used gold clusters with up to 58 atoms to simulate the adsorption site. The equilibrium distances between the adatoms and the gold surface and the corresponding binding energies were calculated using the non-collinear two-component RDFT formulation [36]. The stability of the net Bader charge of SHE atom and the neighboring Au atoms with respect to increase of n indicated the cluster size used was appropriate. The resulting desorption energies estimates lie within the 1.0 – 1.2 eV range for E113 [34] and 2.50 eV for E120 [35], being substantially lower than previously reported values, obtained from simple semiempirical models (1.65 eV for E113 [37] and 3.67 – 3.71 eV [35, 38] for E120). More accurate RDFT desorption energies estimates can be used to parametrize semiempirical models.

4. CONCLUSIONS

Experimental data on the chemical properties of SHEs with atomic numbers of 112 and higher include only few events of gas thermochromatography. The correct and detailed interpretation of the available experimental data cannot be performed without using theoretical modeling. The criterion of the reliability of these models, along with the evident requirement of the reproduction of experimental data (which may be accidental due to the sparsity of the latter), is the agreement between the results obtained with the use of different theoretical approaches. Two-component density functional theory in its non-collinear formulation combined with the accurate relativistic electronic structure model defined by shape-consistent small-core pseudopotentials (RDFT/PP) provides a robust basis of efficient computational schemes for predicting energetic and structural properties of complex polyatomic systems including superheavy elements. However, since the direct first-principles simulation of thermochromatographic experiments is possible only in the frames of RDFT, the estimation of the reliability of these methods and the elucidation of the scope of their applicability are worthy of particular attention.

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