

Effect of nuclear charge distributions on electronic orbitals in superheavy elements

J. Jose^{1,*}, M. Gupta¹ and Y. K. Gambhir^{1,2}

¹Manipal Centre for Natural Sciences, Manipal University, Manipal- 576104, INDIA

²Department of Physics, IIT Bombay, Powai, Mumbai-400076, INDIA

* email: jobin.jose@manipal.edu

Introduction

Modern relativistic quantum many-body theories are able to predict atomic properties with a high degree of accuracy. However the effect of the choice of nuclear charge distributions on the valence orbitals, which play a critical role in deciding the chemical properties of superheavy elements (SHE), needs to be better understood.

The Multi-configuration Dirac-Fock (MCDF) technique [1] has been successfully applied to investigate electronic structure properties. In most of these calculations, nuclear effects are taken into account by assuming either a point nucleus or an extended nuclear charge distribution (*e.g.* Fermi type distribution). As a first step we investigate the effect of a finite nuclear charge distribution on the electronic orbitals. To demonstrate the effect, we consider the SHE Cn ($Z=112$) and the lighter Group 12 element Zn ($Z=30$). These two elements have similar valence electronic shell structure. Moreover, Cn is believed to be the heavier homologue of Zn. Two sets of electronic structure calculations using the MCDF technique are carried out assuming a (1) point nucleus and (2) Fermi nuclear distribution with two parameters, diffuseness and radius. To investigate the effects of nuclear size on electronic properties such as radial probability density, orbital binding energy and relativistic contraction, results obtained from the two sets of calculations are presented and discussed.

Results and Discussion

Fig. 1 shows the comparison of the radial probability density of 1s electrons of Zn and Cn for the two sets of calculations. It is evident from the figure that the finite size of the nucleus pushes the radial probability density to a larger

radius for Cn. However in the case of the lighter atom, Zn, both the point and the Fermi distribution predict the same

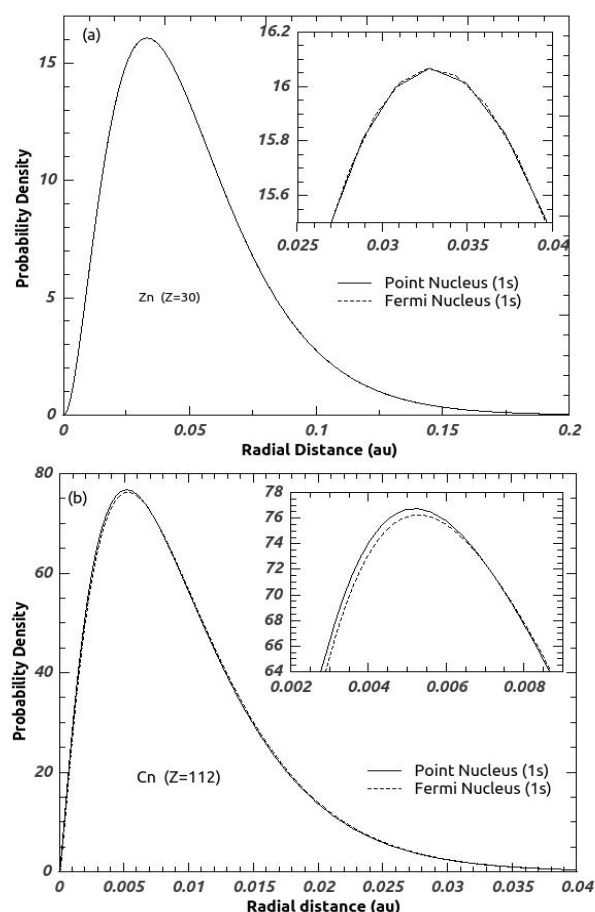


Fig 1: Radial probability distribution of 1s electrons for (a) Zn and (b) Cn, obtained employing point (Solid line) and Fermi (Dashed line) nucleus. Inset shows the radial density of the probability distribution at its maximum.

electronic orbital properties. This difference in the behavior for Zn and Cn is due to the finite size of the heavier nucleus affecting the 1s orbital significantly. A similar observation is made for the valence subshells where the 4s subshell of Zn is relatively unaffected while the outermost 7s subshell of Cn is noticeably influenced by the finite nuclear charge distribution.

Fig. 2 shows the percentage change in the binding energy of orbitals ($l=0$) with the inclusion of a finite nuclear charge distribution for Zn and Cn. For the lighter element, the percentage change in energy is negligible ($\sim 10^{-3}$ %) but for the heavier element it is moderate ($\sim 2\%$). Table 1 indicates the change in the binding energy (%) of orbitals of Cn. We see that the maximum percentage changes are for the s-orbits ($l=0$) as expected. Due to the absence of centrifugal barrier term in the effective potential for orbitals with $l=0$, electrons tend to penetrate the nuclear radius. Therefore the finite size of the nucleus has a greater effect on the s-orbitals.

We have also estimated the percentage relativistic contraction of the valence orbital of Cn with both point and Fermi nuclear charge distributions, which are respectively 32% and 31%. It would be interesting to see the degree to which the difference in the relativistic contraction (1% in this case) can be used to understand the chemical properties of the heaviest elements.

An improved procedure involving a microscopically calculated nuclear charge density distribution is being developed and will be used in future calculations. Work along these lines is in progress.

References

- [1] I. P. Grant, Relativistic Quantum Theory of Atoms and Molecules: Theory and Computation (Springer, Berlin, 2007).

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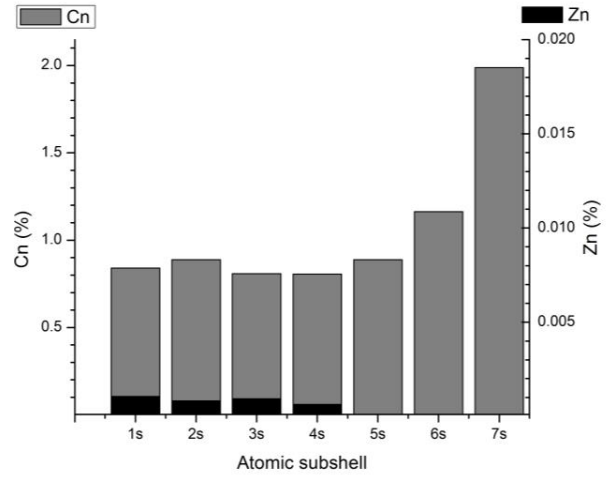


Fig 2: Percentage change in the binding energy with inclusion of finite nuclear distribution in Cn (Left axis) and Zn (Right Axis).

Subshell	Cn
1s	8.40942×10^{-1}
2s	8.87774×10^{-1}
2p	3.7184×10^{-2}
3s	8.08316×10^{-1}
3p	4.45548×10^{-2}
3d	4.48682×10^{-2}
4s	8.05429×10^{-1}
4p	5.79083×10^{-2}
4d	6.24183×10^{-2}
4f	7.83517×10^{-2}
5s	8.87832×10^{-1}
5p	9.12292×10^{-2}
5d	1.15049×10^{-1}
5f	2.70877×10^{-1}
6s	1.16252
6p	2.50108×10^{-1}
6d	7.59192×10^{-1}
7s	1.98872

Table 1: Change in the binding energy (%) of different subshells of Cn with inclusion of finite nuclear distribution