Journal of Physics: Conference Series

Effects of exchange-correlation functionals on the structure and the photoionization dynamics of Na_{40} versus Na_{92} cluster

Effects of exchange-correlation functionals on the structure and the photoionization dynamics of Na_{40} versus Na_{92} cluster

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Synopsis We study the photoionization properties of the Na_n (n=40 and 92) clusters in a spherical jellium frame using the Kohn-Sham density functional method. Two well known form of exchange-correlation (xc) functional in the framework of local density approximation (LDA) with Gunnarsson-Lundqvist parametrization[1] are employed: i) the electron self-interaction correction (LDA-SIC) [1] and ii) the van Leeuwen and Baerends model potential (LDA-LB94) [1].

The structure and photoionization dynamics of Na_n cluster are investigated using density functional theory. The primary objective of the current work is to study the impact of the form of xc in determining its properties by employing LDA-LB94 and LDA-SIC. To the best of our knowledge, not many work have been reported comparing these two schemes.

The real ionic core potential with tightly bound core electrons is replaced by a constant positive background of Na^{10+} ions smeared into a spherical jellium. The Kohn-Sham equation for the delocalized valence electrons ($3s^1$) from each Na atom is solved to obtain the ground state structure of the Na_n in the LDA. The unphysical electron self-interactions in LDA are corrected by using the above mentioned schemes. LDA-LB94 scheme being a prototype of the gradient-corrected class of approximations naturally produces the correct asymptotic behaviour. It is expected to be more realistic than LDA-SIC which removes self-interactions by orbit-by-orbit elimination resulting state-dependent potentials [1].

A time-dependent LDA (TDLDA) with the above two xc forms are used to study the photo response of Na_n clusters. In this method, the photoioinzation cross section is calculated by

$$\sigma_{PI}(\omega) = \sum_{nl} 2(2l+1)\left|\left\langle kl'\left|\delta V(\vec{r'},\omega)\right|nl\right\rangle\right|^2$$

where δV is self-consistent field potential including both the dipole interaction term (z), and the important electron correlation term. Here, nl denotes the occupied state and kl' are dipole-selected continuum.

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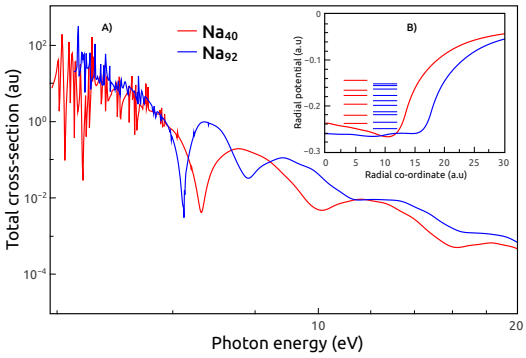

Figure 1. A) Total photoionization cross section B) Radial potentials and energy levels of Na_{92} and Na_{40} using LB94 scheme.

In Fig. 1 is shown the σ_{PI} for Na_{40} and Na_{92} along with the radial potentials and the energy levels (inset figure). The narrow structures at lower energies are the single electron excitations and the diffractive type broad oscillations are found at higher energies in both cases. It is to be noted that the oscillations shortened with increasing size of the cluster. These profiles will be compared with corresponding LDA-SIC results and will be presented in the conference. This work is partially supported by the NSF-USA grant PHY-1806206.

References

[1] Choi J *et al* 2017 *Phys. Rev. A* **95** 023404 and references therein.