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Far above threshold confinement resonances in A@C_{60}^z atoms

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Synopsis It is established, that confinement resonances in the photoionization of an nl subshell of the atom A confined in either neutral or charged C_{60} may be significant even at photon energies far above the nl ionization threshold, contrary to the existing expectations. Reasons are given. Proof is presented.

Resonances, termed confinement resonances (see, e.g., [1] and references therein), in an nl photoionization cross section of the atom A encapsulated in the hollow cage of neutral ($z = 0$) or charged ($z \neq 0$) C_{60}^z ($A@C_{60}^z$) [1, 2], have attracted much attention in recent years. The resonances occur due to the interference of photoelectron waves emerging directly from the nl subshell, and those scattered off the C_{60}^z confining potential. These resonances have been known to diminish rapidly just a few tens eV away from the I_{nl} ionization threshold. Correspondingly, the nl photoionization cross section $\sigma_{nl}^{A@C_{60}^z}(\omega)$ of the confined atom and that of the free atom $\sigma_{nl}^{A}(\omega)$ have been thought to be nearly the same in the high energy end of the spectrum.

The aim of this paper is to demonstrate, that confinement resonances may be significant even far above the threshold energies, contrary to expectations. To scrutinize the high energy end of the spectrum, we employ the recent concept of correlation confinement resonances [1]. In addition, in certain instances, we combine this concept with the fact [3] that interchannel coupling between an nl subshell ionization amplitude with $l > 0$ and amplitudes of inner subshells with $l' < l$ generally must be very important above the $n'l'$ threshold. As a result, we discover, that sizable confinement resonances may revive in $\sigma_{nl}^{A@C_{60}^z}(\omega)$ far above the nl threshold.

In the study, the C_{60} cage is modeled by a square-well potential, as in Refs. [1, 2]. Interchannel coupling is accounted for in the RPAE methodology [4]. The Ne $2p$ photoionization of $Ne@C_{60}^{1-}$ as well as the Ba $5s$ photoionization of $Ba@C_{60}$ are chosen as case studies. The calculated results are displayed in Fig. 1.

One can see from Fig. 1, that there is a strong resonance in the Ne $2p$ photoionization cross section of $Ne@C_{60}^{1-}$ around $\hbar\omega = 890$ eV. This resonance, positioned nearly a thousand eV above the $2p$ threshold, is a confinement resonance. It is induced by a $1s$ near threshold confinement resonance in $\sigma_{1s}^{Ne@C_{60}^{1-}}(\omega)$ [2] via the interchannel coupling with the $2p \rightarrow \epsilon s, \epsilon d$ transitions. Similarly, a sizable resonance oscillation in the Ba $5s$ photoionization of $Ba@C_{60}$ around 120 eV is a confinement resonance which is induced, via interchannel coupling, by a strong confinement resonance in the inner Ba $4d$ photoionization.

Thus, the presented data establish and prove the possibility for revivification of noticeable confinement resonances in the far above threshold photoionization of endohedral atoms A@C_{60}^z.

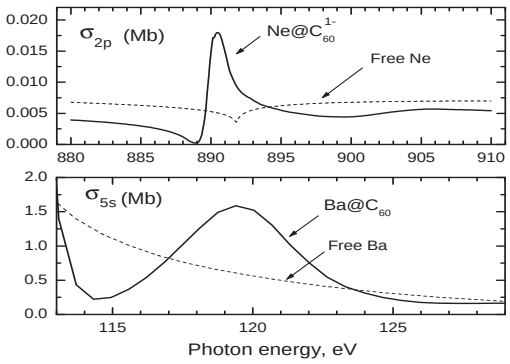

Fig. 1. Calculated photoionization cross sections $\sigma_{2p}^{Ne@C_{60}^{1-}}(\omega)$ and $\sigma_{5s}^{Ba@C_{60}}(\omega)$ far above the $2p$ and $5s$ ionization thresholds, respectively.

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References

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