Binding energies of fullerene and complex atomic negative ions

Alfred Msezane† [1], **Zineb Felfli** † [2]

† Department of Physics and CTSPS, Clark Atlanta University, Atlanta, Georgia 30314, USA

Synopsis A robust potential which embeds fully the vital core polarization interaction has been used in the Regge-pole method to explore low-energy electron scattering from C_{60}, Eu and Nb through the total cross sections (TCSs) calculation. From the characteristic dramatically sharp resonances in the TCSs manifesting negative ion formation in these systems, we extracted the binding energies (BEs) for the C_{60}^-, Eu^- and Nb^- anions. Our BE for C_{60}^- ground state is in outstanding agreement with the measured electron affinity (EA) of C_{60} [1]. For anionic Eu^- and Nb^- our BEs are compared with the measured EAs [2-4].

Progress toward a fundamental theoretical understanding of the mechanism underlying low-energy electron scattering from heavy and complex atoms, including fullerenes, leading to stable negative ion formation has been very slow. The presence of many intricate and diverse electron configurations characteristic of low-energy electron interactions in these systems leads to computational complexity yielding uncertain electron affinities (EAs). The representation of the fullerene cage potential continues to plague theoretical studies as well.

Our Regge pole approach [5], completely new in the field of clusters/fullerenes, should be considered as an investigation toward a fundamental understanding of low-energy electron collisions with fullerenes and complex atoms. The Regge-pole method is appropriate for investigating fullerene negative ion formation as resonances since Regge poles, singularities of the S-matrix, rigorously define resonances. Fully embedded in the Regge pole method are the crucial electron-electron correlations and the vital core polarization interaction. These effects are mostly responsible for the existence and stability of typical negative ions.

Figure 1 exhibits the calculated e-C_{60} TCSs (the inset shows e-Nb TCSs for comparison). Indeed, the TCSs are characterized by Ramsauer-Townsend minima, shape resonances and dramatically sharp resonances corresponding to fullerene anions formation during the collisions. The BE at 2.66 eV (blue curve) agrees excellently with the EA [1] while for Nb the measured EA[4] agrees with our excited state BE of 0.902 eV and not with the ground state BE of 2.48 eV. This has created a quandary.

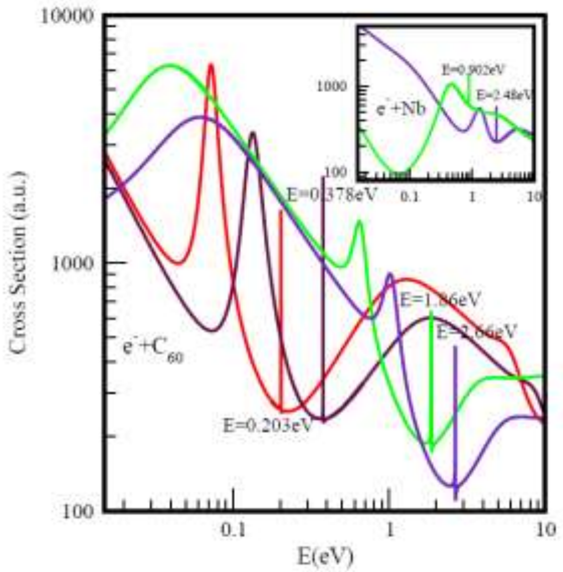

Figure 1: TCSs (a.u.) for e-C_{60} elastic scattering. The blue curve represents the ground state TCS; the other curves correspond to long-lived metastable and excited states. The inset represents TCSs for atomic Nb for comparison.

Research is supported by U.S. DOE, OBES, OS

References

[1] D. –L. Huang *et al* 2014 *J. Chem Phys.* **140** 224315

[2] S. -B. Cheng and A. W. Castleman 2015 *Sci. Rep.* **5** 12414

[3] V. T. Davis and J. S. Thompson 2004 *J. Phys. B* **37** 1961

[4] Z. Luo *et al*. 2016 *Phys. Rev. A* **93**, 020501(R) **93** 020501(R)

[5] D. Sokolovski *et al*. 2007 *Phys. Rev. A* **76** 012705

[1] E-mail: amsezane@cau.edu

[2] E-mail: zfelfli@cau.edu