

Large fullerenes for nanocatalysis, sensors and organic solar cells

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Synopsis We report here on first low-energy electron elastic scattering total cross sections (TCSs) for C₉₄, C₉₆, C₉₈, C₁₁₂ and C₁₂₀ fullerenes calculated using our robust Regge pole methodology. The TCSs are found to be characterized by correlation and polarization induced dramatically sharp resonances manifesting long-lived metastable negative ion formation. We extract the binding energies (BEs) of the resultant anions formed during the collision.

Fullerenes have extensive and crucial applications in science, nanotechnology and industrial research. In particular, in modern organic solar cells the photons absorbed by the donor, usually a polymer create hot-carriers (electrons/holes) which move into the acceptor material, usually a fullerene derivative[1]. Understanding the stability and degradation mechanism of organic solar cells is essential before their commercialization. To overcome the rate of irreversible polymer photobleaching in blend films (polymer: fullerene), designing polymers and fullerenes with larger electron affinity (EA) has been proposed [2]. This has motivated this study to search for fullerenes with larger EAs.

Recently, our robust Regge pole methodology, wherein is fully embedded the electron-electron correlations and the vital core-polarization interaction achieved a theoretical breakthrough in low-energy electron scattering from fullerenes [3]. Entirely new in the field of cluster/fullerene collisions, the Regge pole methodology was benchmarked on the measured EAs of C₆₀ and C₇₀ [4, 5] and used to produce the unprecedented theoretical BEs for the anions C_n⁻ (n=60 through 92) that matched excellently the measured EAs [3].

Here the method has been used to calculate TCSs for C₉₄, C₉₆, C₉₈, C₁₁₂ and C₁₂₀ fullerenes and extract the BEs of the resultant anions. The typical calculated TCSs for the large C₁₁₂ fullerene are displayed in Fig. 1. The results demonstrate that when subjected to varying gentle electron impact energy the investigated fullerenes respond through rich resonance structures, representing doorway states to stable ground anions. These results significantly widen the selection scope of tunable fullerenes for multiple functionalization through their anions. In particular the series of resonances could provide a mechanism for dumping out the hot-carriers thereby eliminate their liability in the efficient operation of robust organic solar cells.

The long-lived metastable resonances support the conclusion that the experimentally detected fullerene isomers correspond to metastable states [6]. We also found

relatively large ground state BEs as high as 3.56 eV for C₉₈⁻ and 3.74 eV for C₁₂₀⁻ anions. Importantly, a single large fullerene such as the C₁₂₀ could replace the Au, Pd and Sn atoms in the catalysis of H₂O₂ from H₂O in the experiments [7] for water purification in the developing world.

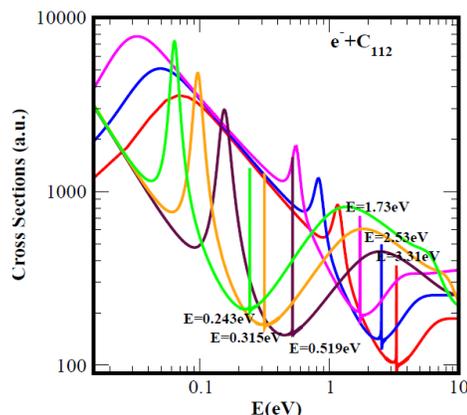


Fig. 1: Total cross sections (a.u.) for C₁₁₂. The red, blue and pink curves represent results for the ground and induced meta-stable (first and second), respectively; the black, orange and green curves are the TCSs for the first, second and third excited states, respectively. Sharp lines represent C₁₁₂⁻ anion formation.

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