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Shrinking diffraction “fringes” in positronium formation from C_{60} to C_{240}

Shrinking diffraction "fringes" in positronium formation from C_{60} to C_{240}

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Synopsis Due to the bulk electron capture from the molecular shell of fullerenes by incoming positron projectiles and a dephasing effect across the shell width, the positronium formation signal yields diffraction fringes in the target recoil momentum space. Our results show the variance in the separation and shape of the fringe pattern as a function of the fullerene size from C_{60} to larger C_{240}.

Varieties of matter have been probed by the positronium (Ps) formation upon bombarding them with positron beams. They range from atoms, molecules, polymers to solids, liquids, surfaces/films, metal-organic-frameworks and embedded nanostructures. However, using nanoparticles as targets in Ps formation can yield novel effects, since solid-like delocalized electrons in nanoparticles are contained in atom-like finite spaces. Fullerenes can be excellent prototypes for such studies. We recently took pilot strides in probing the Ps formation from gas phase C_{60} and predicted a novel diffraction phenomenone that underpins the Ps formation at energies above the C_{60} plasmon excitation [1, 2]. The effect induces fringes in C_{60} recoil momentum which can be called the diffraction resonances. In the present study, we use C_{240} as the diffractor and show the critical dependence of these resonances on the fullerene size.

The structure of a C_{240} molecule is described by the local-density approximation augmented by the LB94 exchange-correlation functional [3]. The positron impact on C_{240} leading to the Ps formation is treated by the continuum distorted-wave-final-state approximation [4].

We compare results of C_{240} in Figure 1(a) as a function of the recoile momentum with those in 1(b) of C_{60}. Results are presented as the ratios of Ps(1*s*) formation cross sections captured from selected states of the target. This facilitates a better representation of resonances by roughly neutralizing the decay of the cross sections. As seen, the fringe separation is almost halved going from C_{60} to C_{240}, in reciprocal proportion of their radii, in analogy to the shrinking fringe pattern with increasing slit size in classical single-slit experiments. Also, the home/homo-1 shape is very different in C_{240} compared to C_{60}.

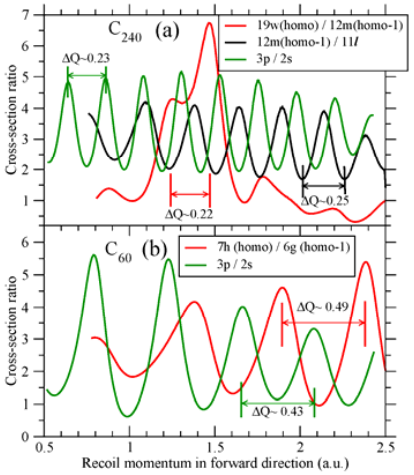

Figure 1. (a) Ps(1*s*) cross section ratios of C_{240}. (b) Same for C_{60}.

The work may encourage experimental applications of Ps formation spectroscopy to gas-phase nanosystems. Supported by the National Science Foundation grant PHY-1806206.

References

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