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Photoionization of neutral magnesium and sodium anion in C_{60} versus C_{240}

Photoionization of neutral magnesium and sodium anion in C_{60} versus C_{240}

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Synopsis We investigate the effects of confinement and electron correlation on the photoemission properties of Mg and Na^- endohedrally sequestered in C_{60} versus C_{240}. Cross sections and Wigner-Smith time delays for emissions from various electronic levels are computed and analyzed in time-dependent local density approximation.

The study of the photoemission in real time using short pulses is key in exploring electron correlations in matter. Technological advents in producing attosecond (*as*) pulses or pulse-trains made it possible to resolve electron dynamics in laser-matter interaction on *as* timescale [1]. For atomic and condensed-phase systems, relative time delays are measured between the photoemission from valence states [2]. Attempts were made to predict the time delays in photoionization process for Ar confined in C_{60} [3]. Here, we perform a comparative study of the effects of electron correlation on the photoionization of Mg and Na^- confined in C_{60} versus C_{240}.

The time-dependent local density approximation (TDLDA) method with the Leeuwen and Baerends (LB94) exchange-correlation functional is employed where the fullerene core is modelled by a spherical jellium shell [4]. We calculate photo cross sections and angle-integrated Wigner-Smith time-delays [3] for atomic-, fullerene- and atom-fullerene hybrid-type levels. We examine the size effects of the molecular cage on the plasmonically enhanced strength of the atomic ionization [5] and the on the routine cavity oscillations. Furthermore, the behavior of emission time delays in *as*, induced by this enhancement as well as by the cavity minima and confinement-modified Cooper minima, as a function of fullerene size is scrutinized in detail.

Figure shows TDLDA cross sections and delays for Mg valence 3*s* emission from C_{60} and C_{240} as a function of the photon energy. Cavity oscillations in the cross sections suggest a reduction in the separation between successive cavity minima from C_{60} to C_{240}. At these minima the correlation effects are dominant which makes the photomission Wigner-Smith delay important. The calculated delays exhibit structures at the minima which, however, are very different from the C_{60} to C_{240} confinement.

The study may open research in spectral and temporal measurements of A@C_{60} and A@C_{240}.

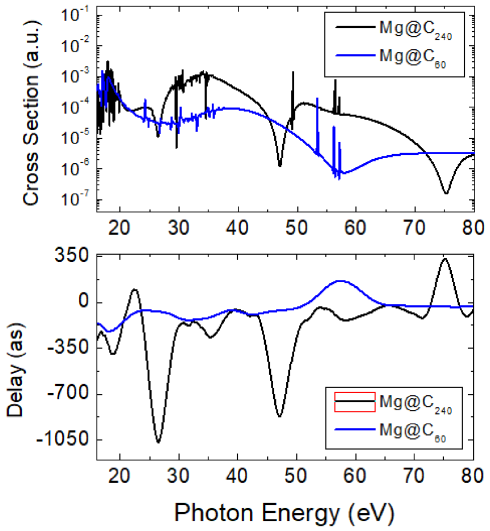

Figure 1. Cross Section (upper) and Wigner-Smith Delay (lower) for the Mg outer 3*s* electron @C_{240} vs @C_{60}.

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