Impact of fullerene polarizability on Wigner time delay in photodetachment of fullerene anions C_N^-

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Synopsis The initial insight into the impact of fullerene polarizability on photodetachment time delay from fullerene anions C_N^- is exposed. The impact is demonstrated to be significant.

Time delay in photoemission of electrons upon photoionization of atoms [1] has become an *ad hoc* topic of many modern studies. To the best of the author's knowledge, no study has been performed with regard to photodetachment time delay from fullerene anions C_N^-. Yet, because fullerenes possess large polarizability, it is interesting to elucidate the impact of polarizability on corresponding photodetachment time delay. It is the aim of the present work to expose the effect of the target polarization on photodetachment time delay from highly polarizable C_N^-s.

To meet the goal, photodetachment time delays from fullerene anions with $N = 60$ and 240 are chosen as case studies. The attached electron is assumed to be a 2p-electron. In view of the complexity of the given many-electron problem, a reasonable simplification of the problem is desirable. In the present work, a popular modelling of a fullerene cage C_N by an attractive spherical potential $U_c(r)$ of certain depth U_0, inner radius r_0 and thickness Δ ([2] and references therein) is utilized. A fullerene anion C_N^- is then formed by the binding of an external electron by this potential into a $n\ell$-state. To account for the impact of the polarization potential V_{pol} of a fullerene on the motion of a released electron, V_{pol} is approximated by a static dipole polarization potential: $V_{pol}(r) \approx -\alpha/[2(r^2+b^2)^2]$ [3]. Here, α is the static polarizability of C_N and b is a parameter of the order of r_0. Thus, a released from C_N^- electron moves in the field of an effective potential $U_{eff}(r) = U_c(r) + V_{pol}(r)$. Then, to determine the sought Wigner time delay $\tau_{n\ell}$, one solves corresponding time-independent Schrödinger equations, finds the electron's initial-state and final-state wavefunctions, calculates the effective photodetachment amplitude $D_{n\ell}$ and its phase $\varphi_{n\ell}$, and completes the study by the calculation of $\tau_{n\ell}$ in accordance with its definition, as an electron-energy derivative of the phase: $\tau_{n\ell} = d\varphi_{n\ell}(E)/dE$ (in atomic units, a.u.).

For illustration, time delays τ_{2p} upon 2p-photodetachment of $C_{60}^-(2p)$, calculated with and without accounting for fullerene polarizability, are depicted in Fig. 1. The latter is self-explanatory, and details of a strong impact of polarizability of C_{60} on time delay are evident.

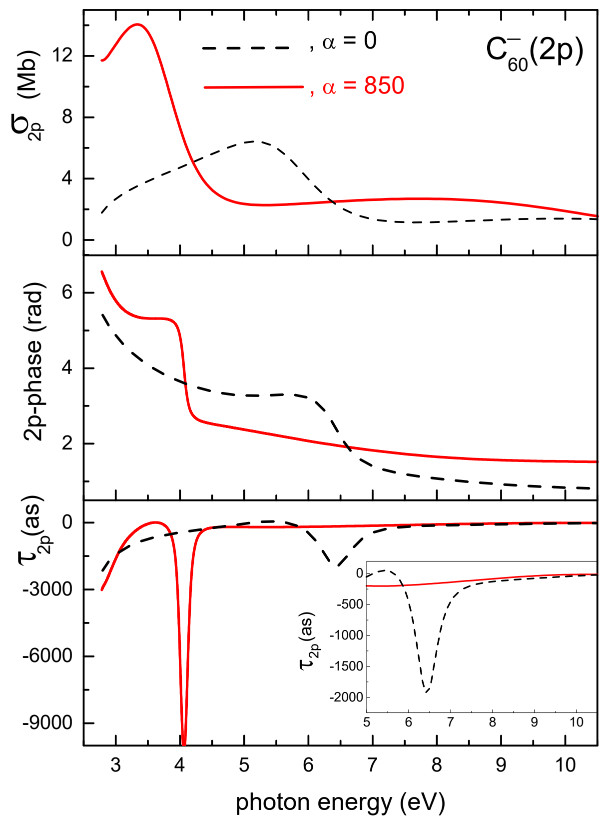

Figure 1. Calculated photodetachment cross section σ_{2p}, phase φ_{2p} and time delay τ_{2p} upon photodetachment of $C_{60}^-(2p)$ with (solid lines) and without (dashed lines) account for C_{60} polarizability α. Parameters: $\alpha \approx 850$, $U_0 \approx -0.26$, $r_0 \approx 5.26$ and $\Delta \approx 2.91$ a.u. [3].

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References

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