

Time-resolved photoemission from endohedral C₆₀ probed by attosecond streaking

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Synopsis We theoretically investigate the time-resolved photoionization of endohedral buckminsterfullerenes as probed by attosecond streaking. We show that the time delays of electrons emitted from the central atom contain the signature of confinement resonances but are also sensitive to molecular near-fields due to enhancement and screening of the probing streaking field by the C₆₀ molecule.

Recent experiments, using either attosecond streaking or the complementary interferometric RABBIT technique, have allowed to study photoemission from rare gas atoms or surfaces in the time-domain with attosecond precision. In this contribution we will study the time-resolved photoionization of endohedral buckminsterfullerenes (A@C₆₀) where a central guest atom A is surrounded by a cage of carbon atoms (C₆₀). Endohedral fullerenes have been the focus of recent time-integrated experiments [1] and *confinement resonances*, due to the interaction of the emitted electrons from the central atom with the quantum well formed by the C₆₀ atoms, have been identified.

It can be expected that the confinement resonances will also leave their signature in the time domain when the ionization process from A@C₆₀ is probed by the attosecond streaking technique [2]. However, in this complex system additional effects due to the interaction of the probing IR field and transport through the cage have to be accounted for. In particular, the 240 valence electrons in the C₆₀ shell feature a high dipole polarizability resulting in an effective screening of the streaking field inside the fullerene and an enhanced dipolar near-field outside the “polar caps” of C₆₀ (Figure 1). The near-field alters the read-out of timing information two-fold: the photoelectron departing from the central atom is effectively subject to the probing streaking field only after passing through the C₆₀ shell. Arrival in the streaking field is thus delayed compared to the ionization of a free atom by the travel time to the surface of the shell. Furthermore, after leaving the shell, the photoelectron experiences the locally dipole-enhanced field instead of a spatially homogenous streaking field.

In our theoretical approach, we simulate the ionization of A@C₆₀ by solving the time-dependent Schrödinger equation (TDSE) using a

suitable model potential representing the static C₆₀ cage [2]. The response of the fullerene to the IR field is calculated using time-dependent density functional theory (TDDFT).

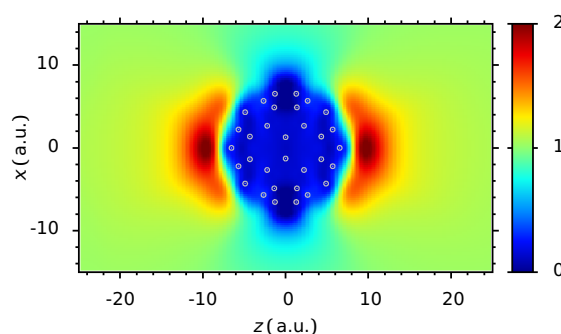


Figure 1. Local streaking field near C₆₀ calculated using TDDFT. The positions of the C atoms are indicated by the grey circles.

The resulting time-dependent near-field is then used in the solution of the TDSE for the emitted electron. We show that the time delays extracted by attosecond streaking contain the temporal signature of confinement resonances but contain also information on the electron transport through the cage and on the near-field enhancement. We identify the separate contributions with attosecond precision.

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References

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