

Photoionization of Xe inside a C_{60}^+ cage: a single-molecule electron interferometer

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Synopsis Absolute cross sections are reported for double photoionization accompanied by loss of n C atoms ($n = 0, 2, 4, 6$) of endohedral $Xe@C_{60}^+$ molecular ions in the photon energy range 60 – 150 eV. The experimental data show clear evidence of confinement resonances arising from interference of outgoing $4d$ photoelectron waves.

Carbon cages can encapsulate atoms and form endohedral fullerenes such as $Xe@C_{60}$. The high symmetry and exceptional stability of such molecular systems are of great multidisciplinary interest [1]. Novel quantum effects are associated with photoionization of an atom located inside a spherical shell. Multi-path interference of photoelectron waves arising from the encaged atom and transmitted or reflected by the carbon cage results in confinement resonances. A first experimental hint to such interference was found by Kilcoyne *et al* [2] in a merged-beam study on photoionization of $Xe@C_{60}^+$ ions. This proof-of-principle experiment has been much improved by employing optimized implantation schemes for sample production using isotopically pure ^{136}Xe atoms. Cross sections for processes



($n=0,2,4,6$) could be measured with greatly improved statistics.

In the investigated photon energy range ionization of a $4d$ electron in the Xe atom is the predominant process and the resulting Xe^+ ion with its $4d$ vacancy favors relaxation by Auger decay. The total oscillator strength f of the ten $4d$ electrons is concentrated in $4d \rightarrow \epsilon f$ transitions leading to a broad maximum in the cross section of the free Xe atom. This 'giant resonance' is most prominent in the net double ionization of the Xe atom and the cross section is known to be associated with roughly two thirds of the total $4d$ oscillator strength ($f=10$). When the Xe atom is encapsulated in a C_{60} shell the giant resonance is substantially distorted and instead of a smooth peak the cross section shows the effect of confinement resonances. The results are displayed in figure 1.

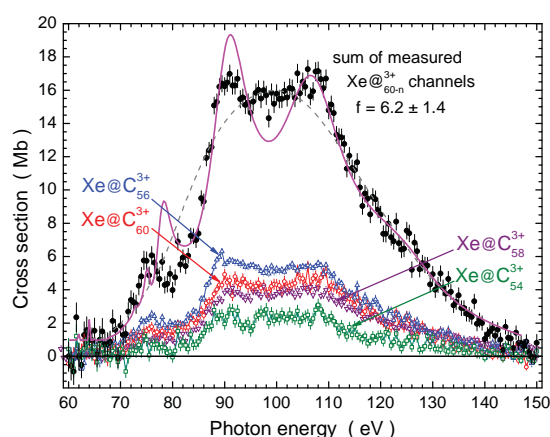


Figure 1. Net Xe $4d$ contributions to double photoionization of $^{136}\text{Xe}@C_{60}^+$ accompanied by the loss of 0, 2, 4 or 6 C atoms. The total oscillator strength associated with the sum is $f = 6.2 \pm 1.4$, i.e., about two thirds of the expected sum over all possible final channels ($f=10$). The recent calculations by Gorczyca and Ballance [3] shown for the free Xe atom (dashed line) and for the endofullerene (solid line) have therefore been scaled by a factor 0.62.

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