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Multi-center interference effect on (e, 2e) electron momentum spectroscopy

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Synopsis The multi-center interference effect of three outermost molecular orbitals (MOs) of CF_4 is investigated using (e, 2e) electron momentum spectroscopy. We show that the observed oscillations are directly informative of the nature of molecular structure. By fitting the experimental results, the bond length of F-F of gas phase CF_4 is determined.

The wave-particle duality is one of the fundamental concepts of quantum mechanism. The wave like particle behaviors were mostly demonstrated through Young's double-slit experiment, in which the coherent addition of different outgoing amplitudes will present interference. The molecular double-slit interference, which was first proposed by Cohen and Fano [1] in 1966, provide a new way to investigate quantum interference effect in molecular scale. In 2003, Stia et al [2] suggested the interference in molecular (e, 2e) process in which the interference originate from the coherent addition of ionization amplitude from different atom centers, as shown in the inset of Figure 1.

For CF_4, the three outermost MOs (1e, $4t_2$, $1t_1$) are composed by $2p$ lone-pair electrons on fluorine atoms. For these MOs consisting of the F $2p$ atomic orbitals, the TDCS, $\sigma_{\rm EMS}(p)$, can be expressed as [3],

$$\sigma_{\rm EMS}(p) \propto \sigma_{\rm A}(p)[1+C_0 j_0(pR_{FF})+C_2 j_2(pR_{FF})], \quad (1)$$

where $\sigma_{\rm A}(p)$ is the TDCS of $2p$ orbital of F atom. j_i $(i = 0,\ 2)$ are the spherical Bessel functions of order 0 and 2 and C_i $(i = 0,\ 2)$ are the corresponding coefficients. R_{FF} is the internuclear distance between the F atoms. Obviously, the interference effect is presented in the last part of e.q. (1). To present the oscillation directly the theoretical TDCS of F atom is divided,

$$\sigma_{\rm EMS}(p)/\sigma_{\rm A}(p) \propto [1+C_0 j_0(pR_{FF})+C_2 j_2(pR_{FF})]. \quad (2)$$

In e.q. (2), $\sigma_{\rm A}(p)$ for the $2p$ orbital of F atom is calculated by distorted wave Born approximation employing B3LYP/aug-cc-pVTZ wave function. The interference factor for the three outermost MOs in large momentum range of CF_4 are shown in Figure 1. It is immediately clear that the experiments exhibit oscillatory structures. The interference factor, $h[1 + C_0 j_0(pR_{FF}) + C_2 j_2(pR_{FF})]$ is employed as a fitting curve for $4t_2$ to reproduce the experiment with R_{FF}, h, C_0, and C_2 being fitting parameters. The best fit to the experiment is presented in Figure 1 (b) by the dashed line. The value of R_{FF} is 3.9 Bohr which is in excellent agreement with 4.07 Bohr reported by electron diffraction[4].

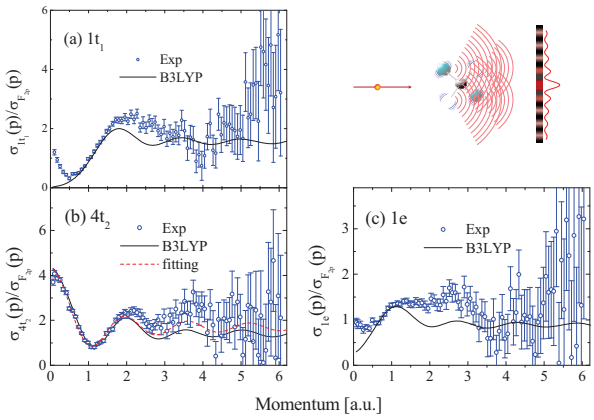

Figure 1. Experimental and theoretical interference effects. (a) $1t_1$, (b) $4t_2$, and (c) 1e molecular orbitals of CF_4.

References

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