

Abstract Submitted  
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**Optical detection of highly delocalized superorbitals in fullerenes<sup>1</sup>**

GUOPING ZHANG, YIHUA BAI, Indiana State University, THOMAS F. GEORGE, University of Missouri-St. Louis — Superatom molecular orbitals (SAMOs) in C<sub>60</sub> are a group of highly delocalized orbitals, extending several nanometers outside the carbon cage, but unfortunately they are hard to detect optically. Here we employ three independent first-principles methods to show that the optical detection of SAMOs is possible for the multiphoton excitation, where successive absorptions of photons boost the optical cross section. In the case of the  $1f$  orbital, we find that our theoretical photoelectron angular distribution matches the unpublished experimental one quantitatively. Experimental confirmation of our prediction will help explain why the mysterious 4-nm separation between C<sub>60</sub> and organic compounds is essential to the efficiency of all the fullerene-based organic solar cells.

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