

Abstract Submitted
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Exploring the Vibrational Stark Effect in Fullerene and Derivatives from First Principles PETER DOAK, Department of Chemistry, UC-Berkeley; Molecular Foundry LBNL , YAJING LI , DOUGLAS NATELSON, Department of Physics, Rice University, LEEOR KRONIK, Department of Materials and Interfaces, Weizmann Institute of Science, JEFFREY NEATON, Department of Physics, UC-Berkeley; Molecular Foundry, LBNL — Fullerene (C60) and its derivatives have played a central role in molecular and organic electronics, where its electron affinity and high symmetry result in key functionality. Understanding the impact of local fields on C60 properties in situ is of considerable interest, and here we determine how electric fields alter vibrational modes via the vibrational Stark effect. Using density functional theory-based finite-difference approach, we calculate the shifts in mode energy and symmetry in electric fields in gas-phase C60, PCBM, and other derivatives of fullerene. We examine the effect of high and low symmetry electronic field orientations, symmetry breaking functionalization, and doping on the the magnitude and mode-dependence of the vibrational Stark effect. The implications for fullerene-based materials under device conditions is discussed. This work is supported by DOE and computational resources were provided by NERSC.

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