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First-Principles Studies of the Vibrational Stark Effect in C60 PETER DOAK, Department of Chemistry, UC-Berkeley, Molecular Foundry, LBNL, YAJING LI, DOUGLAS NATELSON, Department of Physics and Astronomy, Rice University, LEEOR KRONIK, Department of Materials and Interfaces, Weizmann Institute of Science, JEFFREY NEATON, Molecular Foundry, LBNL — C60 has played a central role in molecular and organic electronics, where coupling between charge and vibrational degrees of freedom is of paramount importance. Recent surface-enhanced Raman scattering (SERS) studies of C60-Au junctions have reported significant shifts in vibrational mode frequencies with applied bias. Here we compute the magnitude of the vibrational Stark effect in gas-phase C60 and seek to understand and simulate the shifts in Raman mode frequencies observed in these electromigration junction-SERS experiments. Using density functional theory and a finite-difference approach, we calculate trends in the vibrational Stark effect for different modes of gas-phase C60, comparing directly to experiment and assessing the role of substrate-induced charging and external electric fields. This work supported by DOE and computational resources provided by NERSC.

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