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Raman spectroscopy of the interfacial charge transfer between C60 and gold CHRISTOPHER PYLES, ALEXEY ZAYAK, Bowling Green State Univ — Surfaced Enhanced Raman Spectroscopy (SERS) is a significant extension of the conventional Raman method, which utilizes the fact that molecules absorbed on metal surfaces dramatically increases the Raman scatterings. While the conventional Raman can be used only with large quantities of materials, due to its very small scattering cross section, SERS allows for almost single-molecule measurements. However, along with the useful enhancements, SERS also brings changes to the spectra of molecules. One main example is the shifting of vibrational frequencies. In particular, there is experimental data of this effect for C60 molecules adsorbed on a gold surface. Curiously, not all peaks shift, only a subset. There is a hypothesis that the metal involved in SERS shares electric charge with the molecules in question, which in turn causes the change of frequency. In this work, we use Density Functional Theory (DFT) to computationally find what charge does to the Raman spectrum of a molecule and why only certain vibrations exhibit these changes. Results of this study should help to fully understand the mechanics behind SERS.

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