Abstract Submitted
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Path integral investigation of the electronic spectra of He-tetracene clusters HEATHER D. WHITLEY[1], Lawrence Livermore National Laboratory, Livermore, CA 94551, K. BIRGITTA WHALEY, Department of Chemistry and Kenneth S. Pitzer Center for Theoretical Chemistry, University of California, Berkeley, CA 94720 — Planar aromatic molecules (PAMs) are nanoscale precursors to bulk graphite. Their electronic spectra have been extensively studied in ^{4}He nanodroplets and show a number of unusual spectroscopic features. We have conducted many-body quantum simulations of tetracene in He nanodroplets to probe the 1.1 cm^{-1} spectral splitting of the electronic origin seen for this PAM. We calculate spectral shifts and He density profiles via path integral quantum Monte Carlo simulations. The spectral splitting is examined using a path integral correlation function approach to determine the lowest-lying vibrational excitation frequencies for small He_N-tetracene clusters. Simulations in the S_1 state of tetracene utilize a semi-empirical perturbative interaction potential for a He atom with a PAM. Results for the splitting of the electronic origin and the spectral shifts are in good agreement with experiment. Prepared by LLNL under Contract DE-AC52-07NA27344.

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