Strong Correlation Effect in Fullerene Molecules and Solids

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We report quantum Monte Carlo plus Cluster Perturbation Theory calculations of spectral functions and density of states of fullerene molecules and solids (C_{60}, C_{36} and C_{20}), defined by the standard Hubbard model. By considering the on-site Coulomb interaction U, we find that it plays a vital role in the appearance of energy gaps in the spectral functions and density of states. Our theoretical results are compared with photoemission spectroscopy and scanning tunneling spectroscopy, which, in turn, helps to determine the parameters in the model.