Abstract Submitted
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Correlation-bound anion states[1] VAMSEE VOORA, KENNETH JORDAN, University of Pittsburgh — In a correlation-bound anion, the excess electron is bound to the molecule in a diffuse non-valence orbital and electron correlation is crucial for the electron binding. Examples of such anions include Xe_n^- clusters and certain $(H_2O)_n^-$ clusters. Using many-body methods we have characterized correlation-bound anion states of C_{60}, C_6F_6 and several large acenes. The correlation-bound anion states of these species are related to the image potential states of graphene. Modeling correlation-bound anion states presents challenges for *ab initio* approaches. Hartree-Fock based approaches such as MP2 and CCSD fail to describe these states. The key to treating these species theoretically is to employ a method that allows the singly occupied orbital to relax in the presence of the long-range correlation effects. A model potential approach accounting for image effects for describing the binding of the excess electron will be presented for C_{60}.

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