Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Theoretical studies of nonvalence correlation-bound anions[1] VAMSEE VOORA[2], KENNETH JORDAN, University of Pittsburgh — Nonvalence correlation-bound anion states have been investigated using state-of-the-art ab initio methodologies as well as by model potential approaches. In nonvalence correlation-bound anion states the excess electron occupies a very extended orbital with the binding to the molecule or cluster being dominated by long-range correlation effects. Failure of conventional Hartree-Fock reference based approaches for treating these anionic states is discussed. Ab initio approaches that go beyond Hartree-Fock orbitals, such as Green's function, and equation-of-motion methods are used to characterize nonvalence correlation-bound anion states of a variety of systems including C_{60} and C_6F_6. Edge-bound nonvalence correlation-bound anionic states are established for polycyclic aromatics. Accurate one-electron model potential approaches, parametrized using the results of ab initio calculations, are described. The model potentials are used to study nonvalence correlation-bound anion states of large water clusters as well as "superatomic" states of fullerene systems.

[1] V. K. Voora, and K. D. Jordan, *Nano Lett.*, **2014**, *14* (8), pp 4602-4606.

[1]Travel support through New Investigator Travel Award from Division of Chemical Physics (APS) and NSF grant CHE-1111235 are greatfully acknowledged.
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Date submitted: 12 Nov 2014 Electronic form version 1.4