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Bonding and Electronic Structure of Cluster Assemblies with Metal Carbonyls[1] MEICHUN QIAN, ARTHUR REBER, SHIV KHANNA, Department of Physics, Virginia Commonwealth University, SUKHENDU MANDAL, HECTOR SAAVEDRA, Department of Chemistry, The Pennsylvania State University, PAUL WEISS, Department of Chemistry, The Pennsylvania State University and California Nanosystems Institute, University of California at Los Angeles, AYUSMAN SEN, Department of Chemistry, The Pennsylvania State University — Understanding the factors controlling the band gap energies of cluster-assembled materials is an important step towards creating nano-assemblies with tailored properties. To this end, we have investigated the band gap energies of cluster assemblies involving arsenic clusters bound to metal carbonyl charge-transfer complexes, $[As_7M(CO)_3]^{3-}$ M = Cr, Mo, W. The binding of a single charge-transfer complex is shown to have a small effect on the band gap energy as the arsenic lone pair orbital and metal carbonyl orbitals are closely aligned in energy, resulting in a gap similar to the original cluster. The band gap energy is also found to be insensitive to the architecture of the assembled material. In the case where two charge-transfer complexes are bound to the cluster, the bottom of the conduction band is shown to be localized on a solvent molecule bound to the metal carbonyl.

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