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Towards Nano-Materials with Precise Control over Properties via Cluster-Assemblies[1] MEICHUN QIAN, ARTHUR REBER, SHIV KHANNA, Department of Physics, Virginia Commonwealth University, Richmond, VA 23284, ANGEL UGRINOV, NIRMALYA CHAKI, SUKHENDU MANDAL, HÉCTOR SAAVEDRA, AYUSMAN SEN, PAUL WEISS, Departments of Chemistry and Physics, The Pennsylvania State University, University Park, PA 16802 — One pathway towards nanomaterials with controllable band gaps is to assemble solids where atomic clusters serve as building blocks, because clusters' electronic structures vary with size, composition, and the charged state. To study the role of architecture in cluster assemblies, we synthesized multiple architectures of As_7^{3-} clusters through controlling the counter-cations. Optical measurements revealed that the band gaps vary from 1.1-2.1 eV, even though the assemblies are constructed from identical cluster building blocks. First principles theoretical studies reveal that the variation is a result of altering the LUMO levels by changing the counter-cations. Additional variation in the gap is found by covalently linking the clusters with species of varying electronegativity to alter the degree of charge transfer. The findings offer a novel protocol for synthesis of nanoassemblies with tunable electronic properties.

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