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The Electronic Structure of Diamondoids: When does a Molecule Become a Nanoparticle? TREVOR WILLEY, Lawrence Livermore National Laboratory, CHRISTOPH BOSTEDT, T. MOLLER, Technische Universitat, Berlin, Germany, J. E. DAHL, S. G. LIU, R. M. K. CARLSON, MolecularDiamond Technologies, Chevron, Richmond, CA, T. VAN BUUREN, R. W. MEULENBERG, E. NELSON, L. J. TERMINELLO, Lawrence Livermore National Laboratory — Methane and diamond are common materials with well-known, but extremely different properties. Fundamental, compelling questions then arise: with sp^3 bound carbon molecules/clusters, at what sizes do diamond-like properties emerge? Pure, defect-free, perfectly hydrogen-terminated diamondoids, from ∼0.5 nm to ∼1 nm, bridge the gap between molecules and nanoparticles. Furthermore, experiments in the gas phase eliminate particle-particle interaction and ensure measurement of pure, pristine, and undamaged molecules. X-ray absorption probes the unoccupied electronic states; the carbon K-edge reveals rich electronic structure in the series methane, cyclohexane, adamantane, diamantane, through to hexamantane. Diamondoids show the emergence of a diamond-like band structure. Using x-ray absorption and soft x-ray emission, we will compare our experimental LUMO/conduction band and HOMO/valence band positions with predicted changes in HOMO-LUMO gap from several calculations.

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