Emerging Property Data on Higher Diamondoids – Relationships to Larger Members of the Diamond Series

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Until recently, diamond materials in the 1 to 2 nm particle-size range were virtually unknown. This size range is comparable to the diameters of fullerenes and many single-walled carbon nanotubes which have properties that are complementary to those of nanodiamonds. Therefore, nanodiamonds of this size are especially interesting to the emerging fields of nanotechnology and nanomaterials. Numerous computational studies suggest that diamond is a prized material for nanotechnological applications, and some suggest that 1 to 2 nm-size diamond particles should show interesting and useful properties, such as quantum confinement and negative electron affinities (possibly making them useful as cold-cathode electron emitters).

Unlike many nanomaterials, higher diamondoids can be isolated and crystallized as pure materials with precisely known molecular structures. Knowing their exact structures and having them in pure form, makes possible the use of higher diamondoids, in rational, reproducible “construction” at the nanometer scale, a goal difficult to achieve with many nanomaterials. Moreover, researchers have recently demonstrated that functionalizing higher diamondoids can be accomplished more readily and with greater specificity than had been thought possible. These advances, arising, e.g., from differences in the localization of carbocations and radical cations in higher diamondoid structures, allow specific placement of derivative moieties, making possible structural modifications and assemble using organic chemical techniques.

The numbers of possible structures and molecular weight classes explode with increasing carbon numbers for larger and larger nanodiamond molecules/particles. Beyond the 2-nm size range. A point is quickly reached where precisely knowable diamondoid/diamond structures are no longer accessible with current technology. We will explore possible property transitions across this boundary.

Studies of the properties of the newly discovered higher diamondoid materials have just begun. Some of these studies are producing surprising results, e.g., recent experimental band-gap measurements on diamondoids containing up to six diamond-crystal cages have generated controversy by contradicting predictions of quantum mechanics calculations. Researchers are beginning to explore the spectral and other properties of higher diamondoids. A picture of the relationships between higher diamondoids and larger members of the diamond series is beginning to emerge.