

Tailoring the electronic properties of molecular nanodiamonds: a modular design approach

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Diamondoids are a class of perfectly size- and shape selectable carbon nanoparticles, with a wide range of interesting properties, such as negative electron affinity and high biocompatibility, and with size-dependent (due to quantum confinement effects) optical properties [1]. This makes them promising candidates for many practical applications, such as for example photon- or electron emitters, and biomarkers.

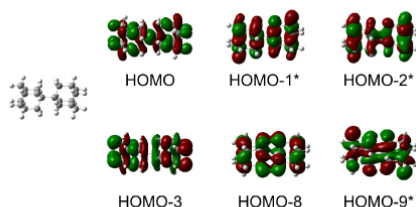
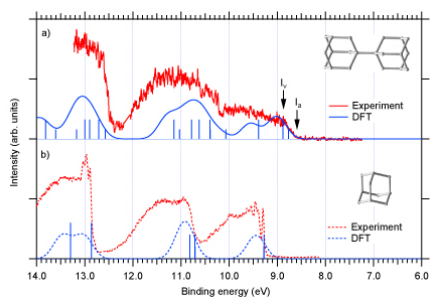


Fig. 1: Photoelectron spectra of adamantane and bi-adamantane, together with the calculated compound valence electronic orbitals.

So far, the isolation and/or synthesis of the higher diamondoids (tetramantane and upwards) has presented a major challenge, since yields are exceedingly small. Recently, the valence electronic structure of functionalized diamondoids has been studied [2], with the conclusion that it is possible to accurately determine orbital ordering and localization in such systems utilizing a combination of experimental and theoretical approaches.

Building on this work, we present a study [3] on whether a modular design principle approach can be utilized to fabricate diamondoid particles, consisting of two or more covalently bonded diamondoid molecules, see fig. 1, that emulate the electronic properties of higher diamondoids. We conclude that depending on the constituent diamondoids and the inter-diamondoid bond order, this is indeed possible. Thus, by using particles made up of smaller diamondoids a new degree of freedom for tuning the band-gap carbon nanoparticles to the visible regime may open up

References:

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