The Electronic Structure of Amorphous Carbon Nanodots

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We have studied hydrogen-passivated amorphous carbon nanostructures with semiempirical molecular orbital theory in order to provide an understanding of the factors that affect their electronic properties. Amorphous structures were first constructed using periodic calculations in a melt/quench protocol. Pure periodic amorphous carbon structures and their counterparts doped with nitrogen and/or oxygen feature large electronic band gaps. Surprisingly, descriptors such as the elemental composition and the number of sp^3-atoms only influence the electronic structure weakly. Instead, the exact topology of the sp^2-network in terms of effective conjugation defines the band gap. Amorphous carbon nanodots of different structures and sizes were cut out of the periodic structures. The calculations predict the occurrence of localized electronic surface states, which give rise to interesting effects such as amphoteric reactivity and predicted optical band gaps in the near-UV/visible range. Optical and electronic gaps display a particle size-dependence similar to inorganic colloidal quantum dots.