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Crystal chemistry and band gaps in polycyclic aromatic hydrocarbons: A dispersion corrected DFT investigation

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The quest for cheap, light, flexible materials for use in electronic applications has resulted in the exploration of soft organic materials as possible candidates, and several polycyclic aromatic hydrocarbons (PAH) have been shown to be versatile (semi) conductors. Dispersion corrected density functional theory is used to explore all crystalline PAHs existing within the Cambridge Crystal Structure Database (CSD) from both structural and electronic standpoints. Excellent agreement is achieved between the experimental and calculated structures, and electronic properties. It was found that addition of a 1.46 eV constant to the Kohn-Sham HOMO-LUMO band gap provided excellent agreement with experiment. Hirshfeld surface analysis revealed that there is a direct relationship between the density of the structures and the relative fractions of C···C intermolecular contacts. Relationships between the contact fractions and the band gap are established. An inverse relationship was found to exist between the density and band gap in these organic molecular crystals (OMC), where the beta and gamma motifs provide the smallest band gaps. Limits in the maximum band gaps of stable PAH crystals containing only aromatic carbon and hydrogen are established as a function of C···C close contact fractions, intermolecular cohesive energy, and density. A 2.0 eV band gap minima was also established for all stable PAH crystals.

Biography

Bohdan Schatschneider completed both his B.S. (1998) and M.S. (2001) in chemistry at Florida Atlantic University. He went on to complete his Ph.D. (2008) at the University of California, Riverside. He is now an Assistant Professor of Chemistry at Penn State University, Fayette where he has published 11 papers in reputed journals and has presented his work 5 times at conference events.

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