



Investigating Electron–Hole Pair Creation and Lifetimes in Amorphous Hydrogenated Boron Carbide



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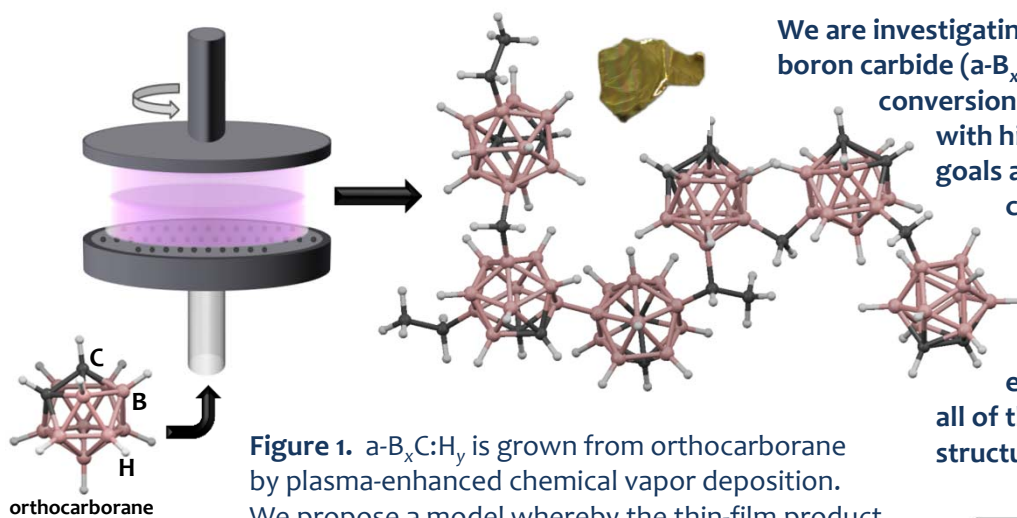


Figure 1. $a\text{-B}_x\text{C:H}_y$ is grown from orthocarborane by plasma-enhanced chemical vapor deposition. We propose a model whereby the thin-film product is composed of an amorphous (disordered) network of partially hydrogenated icosahedra cross-linked via hydrocarbon units.

Accomplishments:

- (1) Growth and characterization of $a\text{-B}_x\text{C:H}_y$ films.
- (2) Development of a model for the local physical structure of $a\text{-B}_x\text{C:H}_y$ using solid-state nuclear magnetic resonance spectroscopy to be used as an input for *ab initio* orthogonalized linear combination of atomic orbitals partial density of state and optical transition calculations.
- (3) Characterization of the electronic structure of $a\text{-B}_x\text{C:H}_y$ through UV and X-ray photoemission spectroscopies prior to two-photon photoemission spectroscopy.

We are investigating the electronic structure of amorphous hydrogenated boron carbide ($a\text{-B}_x\text{C:H}_y$), a material of interest for photovoltaic energy conversion due to its ability to produce electron–hole pairs (ehp's) with high quantum efficiency over a wide energy range. Our goals are to analyze ehp generation theoretically, by calculating the energy levels involved in the photoexcitation process, and empirically, by probing these same energy levels using a specialized two-photon photoemission experiment. We aim to gain a better understanding of where charge is excited from, where it is excited to, what energy gaps are involved, how long the ehp's live, and how all of these characteristics relate to the chemical and physical structure of the material.

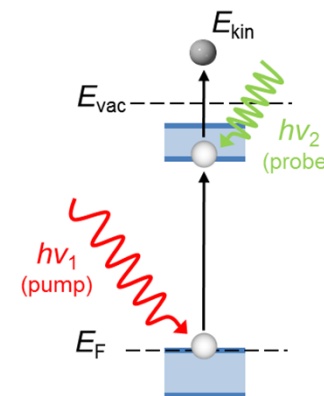
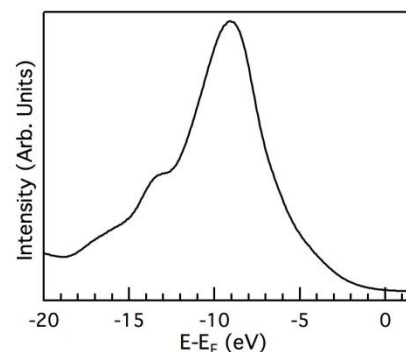


Figure 2. The valence band (from which electrons are removed) of $a\text{-B}_x\text{C:H}_y$ is analyzed through ultraviolet photoemission spectroscopy. Time-resolved two-photon photoemission spectroscopy will allow us to study the unoccupied bands (to which electrons are excited) and the lifetimes of photogenerated electron–hole pairs.