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

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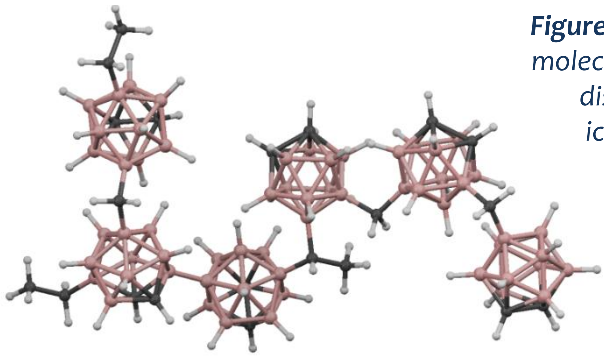


Figure 1. a-B_xC:H_y is a complex molecular solid composed of a disordered network of icosahedral subunits connected by—we hypothesize—hydrocarbon cross-linking groups. Understanding the physical and electronic structure of this nonorthodox material, and their relationship to its transport properties, is a very difficult problem.

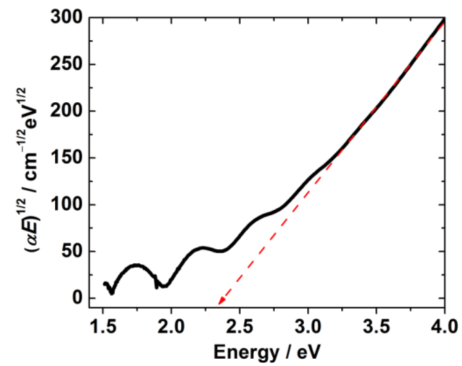
Amorphous hydrogenated boron carbide (a-B_xC:H_y) is of interest for single-junction wideband photovoltaic energy conversion as it has been shown to produce electron–hole pairs (ehp's) over a large energy range with high quantum efficiency. Our objective is to apply a combined computational and experimental approach to investigate the mechanisms responsible for and lifetimes of ehp generation and recombination in thin-film a-B_xC:H_y in the context of its electronic and physical/chemical structure. This study will shed light on the viability of a-B_xC:H_y or similar boron-rich solids as candidate materials for high-efficiency single-junction photovoltaic cells.

ACCOMPLISHMENTS

(1) **Growth and characterization of a-B_xC:H_y films.** Characterization of the atomic composition, density, and some local physical structure details of a-B_xC:H_y films grown by plasma-enhanced chemical vapor deposition.

(2) **Computational modeling of a-B_xC:H_y.** Development and testing of a hybrid method for producing a model with periodic boundary conditions, which applies a gas-phase molecular dynamics condensation scheme to a set of dispersed molecular components followed by an ab initio structural relaxation method. Completion of preliminary density of state and other electronic structure calculations using the crude models thus produced.

(3) **Spectroscopic characterization of the electronic structure of a-B_xC:H_y.** Electronic structure characterization using optical absorption spectroscopy, spectroscopic ellipsometry, X-ray and ultraviolet photoemission spectroscopies, X-ray absorption and emission spectroscopies, and resonant inelastic X-ray scattering measurements.



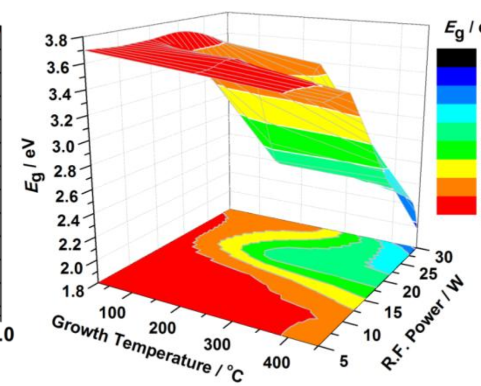
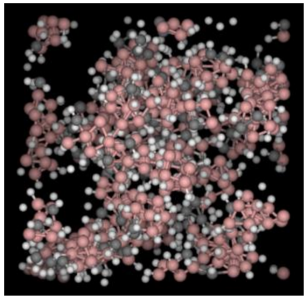


Figure 2. TOP LEFT: Tauc plot derived from the optical absorption spectrum of an a-B_xC:H_y film on glass, used to extract optical band gaps, E_g. TOP RIGHT: Optical band gaps for a series of twenty-four films as a function of growth temperature and power. RIGHT: Periodic amorphous model of a-B_xC:H_y produced using a gas-phase molecular dynamics condensation scheme.



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