

Spectroscopy of B-doped diamonds: experiment vs. theory

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The blue color of diamonds typically arises from ppm amounts of boron that acts as a semiconductor acceptor (*p*-type). This can be compensated by a single N substitution, which acts as an electron *donor*. To contribute to that understanding, the optical absorption spectroscopy of the ‘Hope’ dark blue diamond was measured between 250 and 900 nanometers. In parallel, theoretical first-principles Bethe-Salpeter equation calculations of the optical absorption of substitutionally B-, and N-doped diamond were carried out based on a DFT-relaxed diamond cluster of 64 atoms using ABINIT. Based on this cluster, UV-VIS-NIR optical spectra were calculated that is comparable to that measured for the ‘Hope’ diamond. Briefly, the results show that B-doped diamonds absorb preferentially in the red to NIR range. Based on that result, we can show that the “Hope” diamond is in fact a light blue diamond: its dark blue color arises mostly from its faceting. Application to the “Tavernier Blue” and “French Blue” – two lost historical diamonds - will be presented too.