Abstract Submitted
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Electronic and Optical Properties of Borophene, a Two-dimensional Transparent Metal.[1] LYUDMYLA ADAMSKA, Boston University, SRIDHAR SADASIVAM, PIERRE DARANCET, Argonne National Laboratory, SAHAR SHARIFZADEH, Boston University — Borophene is a recently synthesized metallic sheet that displays many similarities to graphene and has been predicted to be complimentary to graphene as a high density of states, optically transparent 2D conductor. The atomic arrangement of boron in the monolayer strongly depends on the growth substrate and significantly alters the optoelectronic properties. Here, we report a first-principles density functional theory and many-body perturbation theory study aimed at understanding the optoelectronic properties of two likely allotropes of monolayer boron that are consistent with experimental scanning tunneling microscopy images. We predict that despite both systems are metallic, the two allotropes have substantially different bandstructure and optical properties, with one structure being transparent up to 3 eV and the second weakly absorbing in the UV/Vis region. We demonstrate that this strong structure-dependence of optoelectronic properties is present with the application of strain. Lastly, we discuss the strength of electron-phonon and electron-hole interactions within these materials. Overall, we determine that precise control of the growth conditions in necessary for controlled optical properties.

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