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Physical and Thermoelectric Properties of 2-D B_4C Nanosheets¹ ADWAY GUPTA, TATHAGATA BISWAS, ARUNIMA SINGH, Arizona State University — Boron carbide has been well studied both theoretically and experimentally due to its exceptional hardness and use as a high temperature thermoelectric. However, the properties of its two-dimensional nanosheets have not been well established. Here, using van der Waals corrected density-functional theory (DFT) simulations, we show that the bulk B_4C can be cleaved along different directions to form B_4C nanofilms that have low formation energies. We find the dependence of the formation energies on the cleavage planes and surface terminations to be minimal. We also perform a density of states analysis on the bulk using the G_0W_0 method for a more accurate bandgap. Although the density of states of the bulk B_4C reveal that it is a semiconductor with a bandgap of 2.3 eV, the B₄C films are predominantly metallic. We attribute this metallic behaviour to the redistribution of the charges between the B-C bonds at the surface of the films. We find that the Seebeck coefficients of the the B_4C films remain comparable to those of the bulk at varying temperatures. Our work shows that B_4C 2-D films can be synthesised fairly easily along multiple directions, while maintaining near identical thermoelectric properties as that of the bulk.

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