Supplementary Information: Enhancing the Thermoelectric Figure of Merit of BiN via Polymorphism, Pressure, and Nanostructuring

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Materials discovery extends beyond the synthesis of new compounds. Detailed characterization is essential to understand the potential applications of novel materials. However, experimental characterization can be challenging due to the vast chemical and physical spaces, as well as the specific conditions required for certain techniques. Computational high-throughput methods can overcome these challenges. In this work, the transport and thermoelectric properties of the recently synthesized bulk BiN are explored, including the effects of temperature, pressure, carrier concentration, polymorphism and polycrystalline grain size. We find that the band structure is strongly dependent on pressure and the polymorph studied. Both polymorphs exhibit low thermal conductivity at 0 GPa, which rapidly increases when pressure is applied. Electronic transport properties can be finely tuned based on the effects of pressure and polymorph type on the band gap, carrier mobilities, and presence of secondary pockets. The thermoelectric figure of merit can reach values around 0.85 for both p- and n-type BiN if the power factor and lattice thermal conductivity are optimized at 600 K, making this material competitive with other well-known thermoelectric families, such as Bi_2Te_3 or PbX, in the low-to-medium temperature range.

I. ELECTRONIC TRANSPORT PROPERTIES

AUTHOR CONTRIBUTIONS

J.J.P.R and A.M.M conceived and initiated the research project. E.R.R. and V.P. and J.J.P.R performed all calculations and analysis presented in the main text, and wrote the first draft. K. G., A.M.M. and J.F.S. contributed to the data analysis and interpretation. A.M.M. and J.J.P.R supervised the project. All authors discussed the results and contributed to the final paper.

CONFLICTS OF INTEREST

There are no conflicts to declare.

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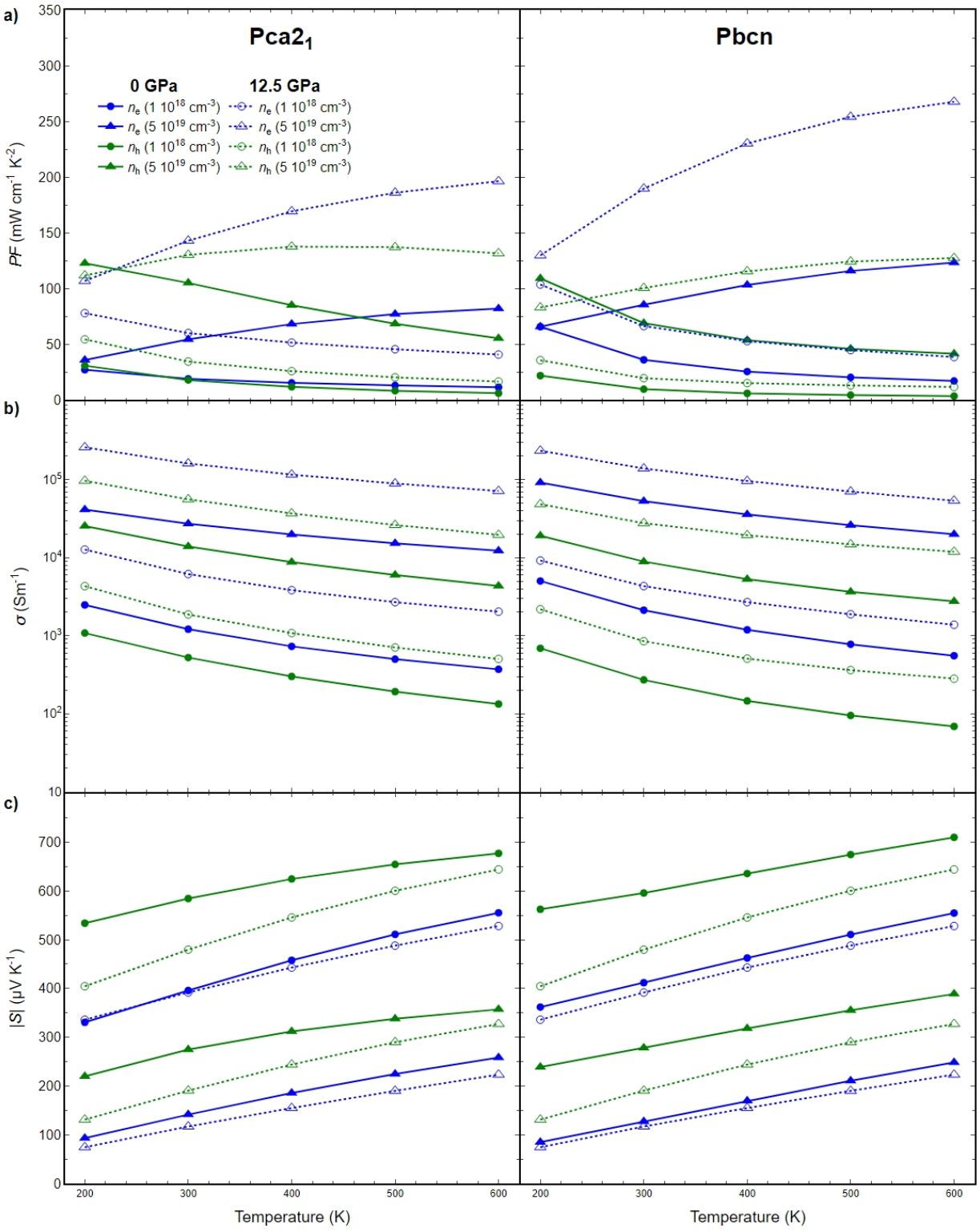

FIG. 1. (a) Power factor (PF), (b) electrical conductivity (σ), and (c) Seebeck coeeficient (S) for Pca2$_1$ (left) and Pbcn BiN polymorph (right). Electronic transport properties are depicted in green and blue for p- and n-type, respectively. Circles and triangles are used for different carrier concentrations. Properties at 0 GPa and 12.5 GPa are plotted in solid and dashed line, respectively.