

Heat Transport in Ultra-Incompressible Carbon Nitrides: A Finite-Temperature Phonon Study

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More than thirty years ago, carbon nitrides featuring 3D frameworks of tetrahedral CN₄ units were identified as one of the great aspirations of materials science, expected to have hardness greater than or comparable to diamond. Here, we investigated the mechanical and thermal transport properties of these new ultra-incompressible carbon nitrides, tI14-C₃N₄, hP126-C₃N₄, and tI24-CN₂. Being wide-band gap semiconductors with intriguing features in their electronic structure, they are expected to exhibit multiple exceptional functionalities besides their mechanical and thermal properties, opening new perspectives for materials science.