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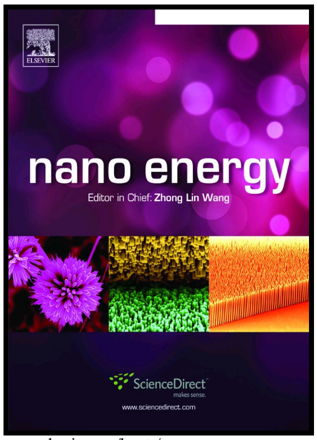

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Bond Saturation Significantly Enhances Thermal Energy Transport in Two-Dimensional Pentagonal Materials

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Abstract

Thermal transport in nanoscale two-dimensional (2D) materials is of great scientific interest and has practical implications for energy related applications like thermal management of energy devices, composite battery materials and on-board thermoelectric power generation for sensors. The abilities to manipulate thermal transport in 2D materials is thus highly desirable for future nano energy technologies. In this work, we identify a general rule for controlling the thermal transport in 2D pentagonal materials through bond saturation. We use first-principles calculations to investigate the phonon properties of a series of pentagonal materials, including penta-graphene (PG), hydrogenated PG (h-PG) and fluorinated PG (f-PG), and find that the bond saturation of the carbon atoms through functionalization can reduce the bond anharmonicity and thus increase the phonon lifetime. We can follow this rule to predict very high thermal conductivity of other pentagonal structures with saturated bonds, including penta-CN_2 (1027 W/mK) and two three-dimensional counterparts of PG called T12-carbon (819 W/mK) and AA T12-