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A theoretical study of 2D AlN on 3D $C_4H_6N_6Ni_2$ clathrate thermoelectric material composites

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ABSTRACT:

Clean and green renewable energy is of paramount importance in the world today. Ab initio calculations using density functional theory demonstrate that superlattice structures can result into lowering lattice thermal conductivity and have improved electronic properties, which result in higher electrical conductivity. It is possible to achieve improved thermoelectricity-generating properties of materials with new superlattices and have large effective mass, as well as density of states at the Fermi level composed of 2D/2D AlN/$C_4H_6N_6Ni_2$. However, higher electrical conductivity requires high-mobility charge carriers, narrow-gap semiconductors and lower electron scattering. Thus, band structure, projected density of state, density of state, as well as spin density of state difference between alpha and beta eigenstates contributions, are used to reveal that heterostructures have advantage over the isolated materials. New superlattice structures would result in improving the charge generation/separation and yield a better thermoelectric material.