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Intrinsic and strain dependent ultralow thermal conductivity in novel AuX (X = Cu, Ag) monolayers for outstanding thermoelectric applications

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A large power factor and ultralow lattice thermal conductivity in 2D-monolayers of AuX (X = Cu and Ag) are achieved *via* first principles calculations. Low phonon frequency, small Debye temperature and high Gruneisen parameter limit the intrinsic thermal conductivity of both the studied materials. An ultra-low lattice thermal conductivity of 0.13 (0.30) W m^{-1} K^{-1} and 0.66 (1.59) W m^{-1} K^{-1} is obtained for unstrained AuCu and AuAg monolayers, respectively, at 700 (300) K, which further reduces to 0.04 (0.09) and 0.26 (0.63) W m^{-1} K^{-1} at 6% biaxial tensile strain. Such values of thermal conductivity are lower than the critical thermal conductivity for the state-of-art thermoelectric materials (k_l < 2 W m^{-1} K^{-1}). The peak values of *ZT* for unstrained monolayers are 2.20 and 1.40, which enhances to 3.61 and 2.91 at 6% strain for AuCu and AuAg monolayers, respectively. Interestingly pudding-mold band textures are found to be responsible for this unusual thermoelectric behaviour. The stability concerns (chemical/dynamic/mechanical) of these monolayers are ensured to stimulate experimental determinations for novel synthesis and possible applications.

1. Introduction

Finding highly efficient thermoelectric materials has been a major struggle in order to address the energy demands and global warming crises. The dimensionless figure of merit ($ZT = \frac{S^2\sigma T}{k}$), which includes the Seebeck coefficient (S), electrical conductivity (e) and total thermal conductivity (k), is frequently used to evaluate the criteria for thermoelectric conversion efficiency.[1] In order to obtain a high value of *ZT*, the focus should be on increasing the power factor ($S^2\sigma$) while decreasing the thermal conductivity.[2,3] These characteristics, however, are inextricably entangled.[2] As a result, obtaining a high *ZT* value remains a significant challenge.

In view of their unique electronic, thermal, optical, mechanical, and transport characteristics, two-dimensional (2D) materials have been a key research area in the last few decades. The database of 2D materials has extended to several hundred after the discovery of graphene. Because of the quantum confinement effect in 2D-thermoelectrics, energy sub-bands in quantum wells are formed which leads to high density of states around the Fermi level and improving the power factor.[4–7] Moreover, due to scattering of phonons by surfaces, the heat conductivity of the lattice significantly drops in low dimensional materials and hence the overall performance of thermoelectric material improves.[8] Many of the 2D materials which have undergone experimental synthesis or predicted theoretically including phosphorene, boron–nitride, and many more attracted pronounced interest in the field of thermoelectricity.[9,10] Such materials provide diverse and phenomenal properties in terms of their composition, strength, charge transfer, bandgap, strain limit, mobility, *etc.* The reported *ZT* value of some of the recent 2D materials such as PbTe (2.9),[11] $ZrSe_2$ (4.26),[12] SnSe (2.51),[13] SnP_3 (3.46)[14] and InP_3 (2.06)[15] is higher than those of their bulk counterparts. M.J. Lee and his co-workers synthesized a 2D layer of SnS_2 and observed a

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