INDIAN INSTITUTE OF TECHNOLOGY GUWAHATI
SHORT ABSTRACT OF THESIS

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SHORT ABSTRACT

Thermoelectric materials that can efficiently convert waste heat into electricity are crucial for sustainable energy technologies. Two-dimensional (2D) materials, owing to their quantum confinement effects and large surface-to-volume ratios, offer new avenues to overcome the coupled nature of transport properties that limit bulk thermoelectrics. Using first-principles density functional theory and Boltzmann transport calculations for electrons and phonons, the present thesis explores design strategies to enhance the thermoelectric figure of merit (ZT) by tuning structural symmetry, surface functionalization, strain, and chemical composition. The structural arrangement is found to strongly affect charge and phonon transport in hexagonal Si–X (X = N, P, As, Sb, Bi) monolayers, resulting in an improved ZT. In Janus MXenes (MM'CO_2), compositional asymmetry and surface modification enhance lattice anharmonicity, reduce lattice thermal conductivity, and improve electronic transport, effects that are further amplified under tensile strain. Similarly, Janus monochalcogenides (M_2XY and MM'X_2; M, M' = Ge, Sn; X, Y = S, Se, Te) exhibit anisotropic band dispersions with high density of states near the band edges and multiple valleys, yielding large directional power factors and enhanced ZT. Finally, in monolayer h-NbN, inclusion of four-phonon scattering processes reveals strong phonon–phonon interactions that drastically suppress κ_l, increasing ZT by 2–3 times to about 1 at elevated temperatures. The study provides fundamental insight into how structural asymmetry, strain, and compositional engineering can be leveraged to optimize thermoelectric performance in 2D materials.