Strain-induced half-metallicity and giant Wiedemann–Franz violation in monolayer NiI_2

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Monolayer NiI_2 has attracted considerable scientific interest due to its unique combination of semiconducting behaviour, strong spin polarization, and complex magnetic ordering, including helimagnetism and multiferroicity at the two-dimensional limit. Recent advances in synthesis and exfoliation techniques have enabled the fabrication of high-quality samples, fostering detailed experimental and theoretical studies. These characteristics position NiI_2 as an excellent platform to investigate the interplay between charge, spin, and heat transport, which is central to thermoelectric and spin-caloritronic applications. In magnetic systems, thermoelectric efficiency can be enhanced through the spin degree of freedom, enabling phenomena such as the spin Seebeck effect, where thermal gradients generate spin currents. Additionally, strain engineering has emerged as an effective and reversible strategy to tune the physical properties of 2D materials. In NiI_2, biaxial strain can modify magnetic phase stability, reshape the electronic band structure, and influence carrier transport, providing a powerful route to optimize thermoelectric and spin-caloritronic performance [1-6].

In this context, in this work we perform a comprehensive density functional theory (DFT) calculation combined with semiclassical Boltzmann transport theory to systematically investigate the electronic, magnetic, and thermoelectric properties of monolayer NiI_2 under biaxial strain. We analyse the energetic competition between ferromagnetic (FM) and antiferromagnetic (AF) configurations, trace the evolution of the spin-resolved band structure, and quantify the strain dependence of key thermoelectric coefficients, including the Seebeck coefficient, electrical conductivity, and power factor. Our findings demonstrate that mechanical strain can induce a semiconductor-to-metal transition in the FM phase, enhance spin-polarized transport, and provide a versatile route to control multifunctional behaviour in NiI_2 monolayers. These results highlight the promise of NiI_2 as a candidate for next-generation spintronic and thermoelectric technologies [7].

References

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