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Band gap closing in multilayer Nickel Bis(ditiolene) induced by interlayer interactions[1] SUCHUN LI, SHEN LI, GANG WU, SHUO-WANG YANG, Institute of High Performance Computing, A*STAR, Singapore — Nickel Bis(dithiolene) shows the highest experimentally recorded electrical conductivity for coordination polymeric materials [JACS 2014, 136, 14357]. On the contrary contrast, the thermal conductivity of such coordination polymeric materials is expected to be very low due to the pores structure. Therefore NiBis and similar coordination polymeric materials are expected to show high thermoelectric figure of merit. Motived by the high potential of this type of materials in thermoelectric applications, we studied Nickel Bis(dithiolene) using first principles calculations. We find very interestingly that monolayer NiBis is a semiconductor with an indirect gap of ˜0.15eV while all multilayer NiBis become metallic. We analyze the underline mechanism using bilayer NiBis with varying interlayer distance, and find that the gap can be gradually opened again by gradually increase the interlayer distance. We reveal that interlayer interactions in multilayer NiBis are more than simple van der Waals interactions. Multilayer NiBis become metallic because of covalent-like interactions between Sulfur atoms across different layers. Making use of this interlayer-interaction mechanism, we can use interlayer distance (pressure) to tune the gap and many related properties such as electrical conductivity, Seebeck coefficient, optical properties, etc.

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