**Thermoelectric properties of HfSe2 monolayer**

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**Abstract**

Recent success of graphene and advancement in the growth of atomically thin layers has led to discovery of new two-dimensional materials. Among vast family of single layer of van der Waals bonded transition metal dichalcogenides, Hafnium Diselenide, HfSe2 has attracted the great deal of scientific attention. Being indirect band semiconductor, HfSe2 layers possess ultra low thermal conductivity resulting it as promising material for thermoelectric applications.

 In this work we present, the detailed investigated the thermoelectric properties of HfSe2 monolayers employing Boltzmann transport formalism. We have presented numerical calculations of electrical conductivity, *σ*, electronic thermal conductivity, *κe*, diffusion thermopower, *Sd*  and thermoelectric figure of merit, *ZT* considering the scattering of electrons from acoustic phonons and charged impurities. We find that HfSe2 monolayer possess extremely low electronic thermal conductivity and relatively high thermopower (~ 100µV/K). Our calculations show that thermoelectric figure of merit is more than 1 at higher temperatures thus making it suitable candidate for thermoelectric applications.



**Figure:** Variation of thermoelectric figure of merit, *ZT* in HfSe2 monolayer.