Theoretical Investigation of Thermoelectric Properties of $NbSe_2$ Polymorphs Based on First-Principles Band Calculations

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Abstract

The flexibility of interlayer stacking sequences in Niobium Diselenide ($NbSe_2$), primarily attributed to the weak van der Waals (vdW) interactions, leads to variations in the electronic properties of the atomic-layered material [1][2]. However, the majority of studies [3] have largely focused on its most stable configuration, $2H_a$, leaving various metastable structures, in particular $2H_c$, 2H-3R, and 3R, rather overlooked. In this study, we conducted first-principles calculations based on density-functional theory (DFT) to investigate the in-plane and out-of-plane thermoelectric properties, including Seebeck coefficient, electrical conductivity, electronic thermal conductivity, and thermoelectric power factor of various polymorphic forms of $NbSe_2$. Employing a semi-empirical Boltzmann transport model revealed that the layered $NbSe_2$ materials exhibit anisotropic transport properties along the in-plane and out-of-plane directions. Aside from a change of sign, the charge density at which the in-plane Seebeck coefficient crosses the zero value varies with the stacking sequence; however, no significant change in amplitude was observed. In contrast, the out-of-plane Seebeck coefficient didn't undergo a sign change, but the amplitude was strongly influenced by the stacking structure. These differences are due to the variations in the electronic structure among the distinct stacking sequences. The results of this work provide an insight into how modifying the stacking configuration could potentially manipulate the thermoelectric properties of nanoscale electronic devices.

References

[1] M. Marezio et al., Journal of Solid State Chemistry, vol. 4, no. 3 (1972) pp. 425–429
[2] H. Moon et al., Nano Energy, vol. 78 (2020) p. 105197
[3] X. Xi et al., Nature Physics, vol. 12, no. 2, (2016) pp. 139-143

Figures

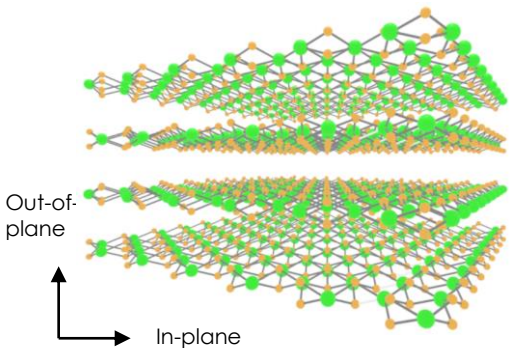

Figure 1: 2H-3R-$NbSe_2$ comprises four layers stacked in repeating sequences of $2H_a$ and 3R phases.

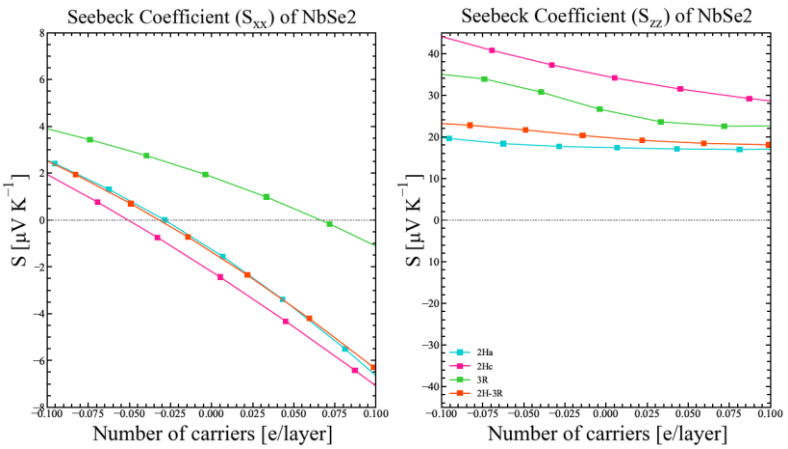

Figure 2: Seebeck coefficient of $NbSe_2$ polymorphs at 300K.