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Phonon Thermal Conductivity of Stanene/hBN van Der Waals Heterostructure

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Supporting Information

S1. Effect of interface interaction scaling factor on the PTC of stanene/hBN.

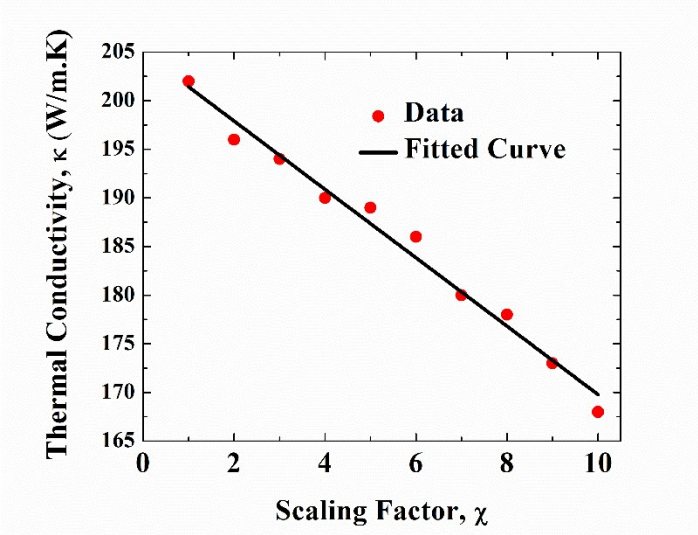

Fig.S1. Variations of PTC of stanene/hBN as a function of scaling factor at 300 K.

The interface interaction strength scaling factor, χ, greatly affects the in-plane phonon thermal conductivity (PTC) of the heterostructure, as reported earlier [1]. To check the effect of interface interaction scaling factors on the PTC of stanene/hBN heterostructure, the scaling factors have been varied up to 10, and corresponding outputs are illustrated in Fig.S1. It has been found that the PTC of stanene/hBN is decreased by ~17.5% as the scaling factor has been increased from 1 to10. When the hBN layer is supported by the stanene layer, the rotation, translation, and reflection factors of each monolayer are notably modified, and the vibrational properties of each monolayer are also altered due to stanene/hBN van der Waals interactions. As the scaling factors increases, the phonon-phonon scattering increases, which eventually reduces the in-plane PCT of the stanene/hBN system [1]. This kind of inverse relation of PTC with increasing scaling factors has been reported for Gr/MoS_2 heterostructure [1].

References

[1] B. Liu *et al.*, "Thermal transport in a graphene-MoS2 bilayer heterostructure: a molecular dynamics study," *RSC Advances*, vol. 5, no. 37, pp. 29193–29200, Mar. 2015, doi: 10.1039/c4ra16891g.