Supporting Information

Investigation for thermoelectric properties of MoS_2 monolayer-graphene heterostructure: density functional theory calculations and electrical transport measurements

Sujee Kim [†,#] Changhoon Lee[‡,ǁ,#] Young Soo Lim[*,⊥] and Ji-Hoon Shim[*,†,‡,ǁ]

[†] Division of Advanced Nuclear Engineering, Pohang University of Science and Technology, Pohang, 37673, Korea

[‡] Department of Chemistry, Pohang University of Science and Technology, Pohang, 37673, Korea

[§] Max Planck POSTECH Center for Complex Phase of Materials, Pohang University of Science and Technology, Pohang, 37673, Korea

[ǁ] Division of Advanced Materials Science, Pohang University of Science and Technology, Pohang, 37673, Korea

[⊥] Department of Materials System Engineering, Pukyong National University, Busan 48547, Korea

# S. Kim and C. Lee have contributed equally to this work

S1) The relative energy as a function of distance between MoS_2 and graphene layer in MoS_2-graphene heterostructure.

In this work, the distance between MoS_2 and graphene layer is 3.3 Å. As shown in figure S1, although 3.35 Å is the equilibrium distance between MoS_2 and graphene layer, the relative energy at distance 3.3 Å and 3.35 Å is smaller than 1meV. So the distance, 3.3 Å, is also reasonable value.

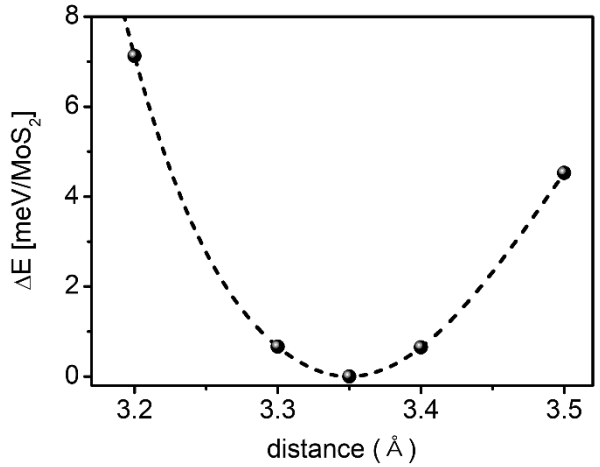

Figure S1: The calculated relative energy ΔE per formula energy of MoS_2 as a function of distance between MoS_2 and graphene layer with vdW+DFT, taking the origin at the lowest energy configuration.