Supplementary Materials for

"Role of modification interlayers in enhancing thermal transport across metal/diamond interfaces"

Xinling Tang[1], Guang Yang[1,*], Zhongkang Lin[1], Yulin Gu[1], Jingfei Wang[1], Xiaoguang Wei[1,2,*]

[1] *Beijing Huairou Laboratory, Beijing 101407, China.*

[2] *China Southern Power Grid Novel Electric Power System (BEIJING) Research Institute Co., Ltd, Beijing, China.*

Supplementary Figures

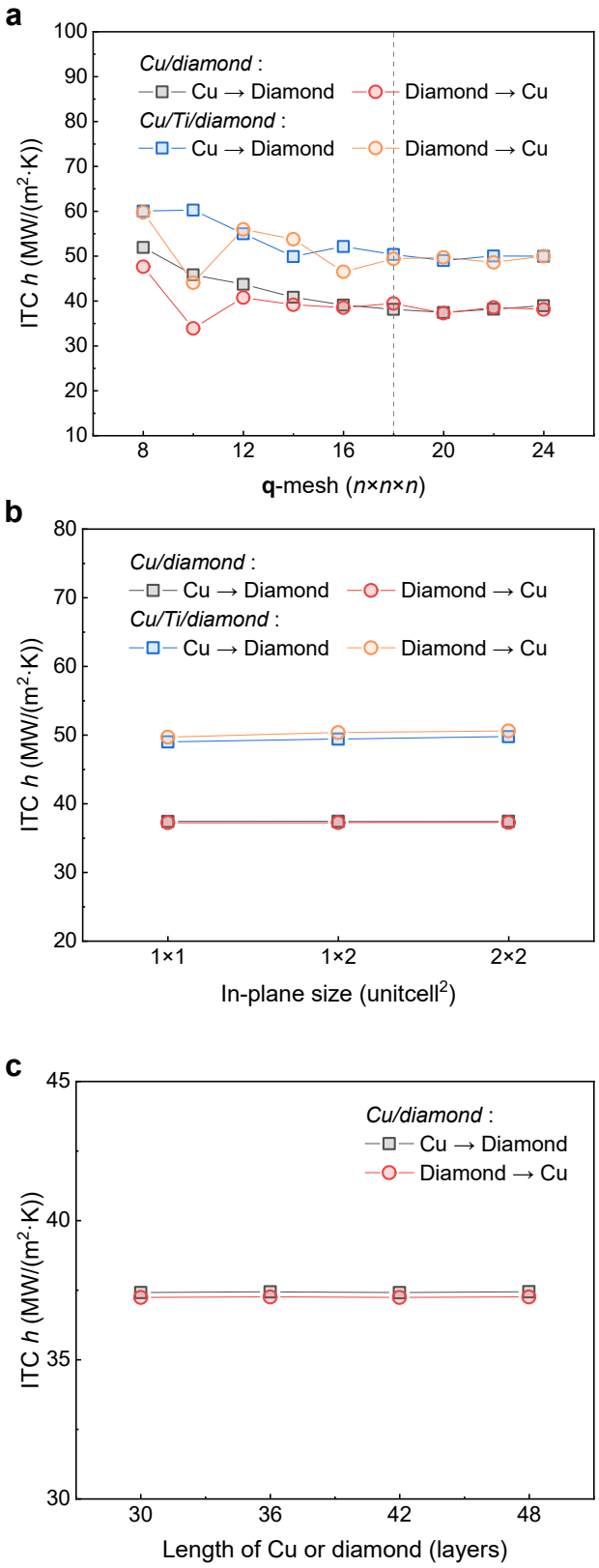

Figure S1. Convergence tests of lattice dynamics simulations against (a) ***q***-mesh of the 1st Brillouin zone, (b) in-plane sizes of models, (c) total lengths of models.

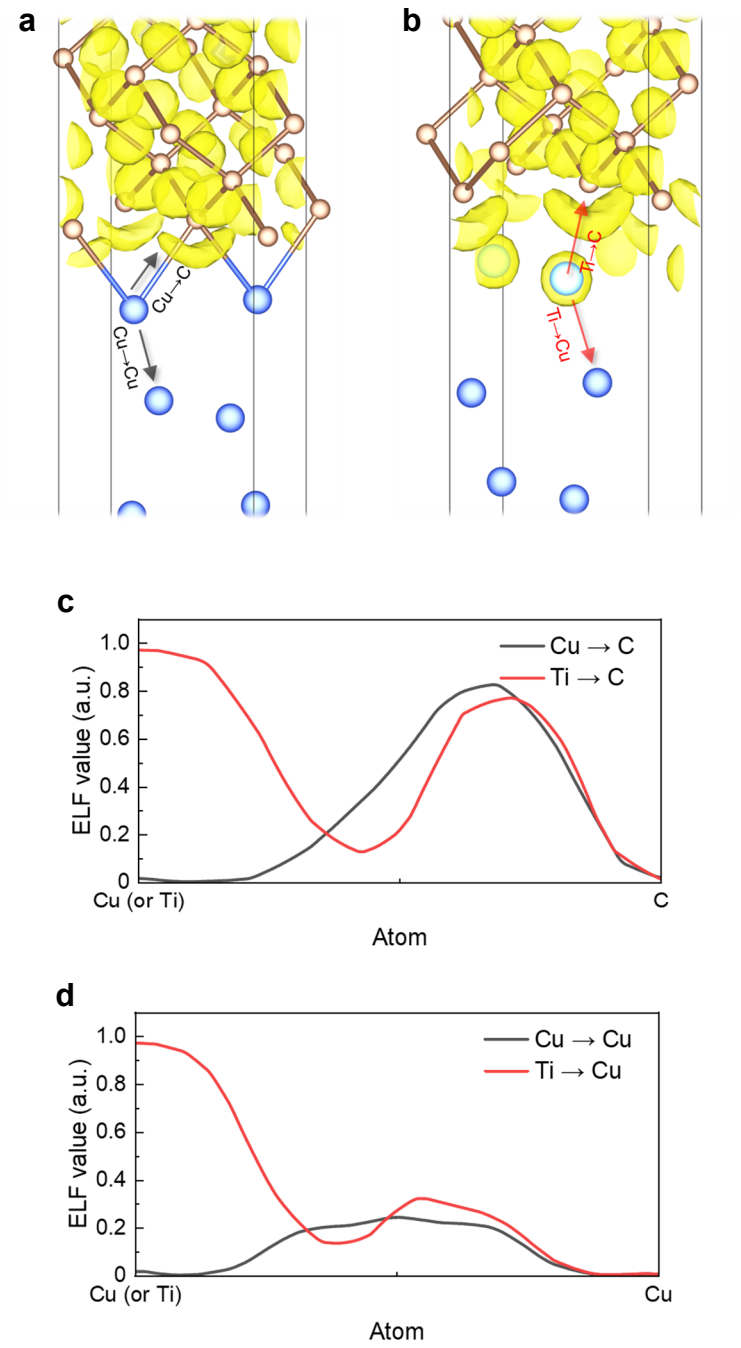

Figure S2. Analyses on the electron localization function (ELF). The ELF isosurfaces at 0.75 of (a) the Cu/diamond interface and (b) the Cu/Ti/diamond interface. There exist lone pairs of electrons around Ti atoms. ELF profiles along (c) Cu → C, Ti → C interactions, (d) Cu → Cu, Ti → Cu interactions.