Electronic Supplementary Materials

Tuning thermal contact conductance at graphene-copper interface via surface nanoengineering

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Density-functional theory optimization details:

To further confirm the bending behavior of graphene nanoribbon (GNR) into the nanogrooves, we perform structure optimization using spin-unrestricted density functional theory (DFT) methods as implemented in the Dmol[3] package.[1,2] The exchange-correlational interaction is computed based on the generalized-gradient approximation (GGA) in Perdew–Burke–Ernzerhof (PBE) form.[3] Double-zeta numerical basis set with polarization functions (DNP)[3] and semi-core pseudopotential are employed to treat the atomic orbitals and core electrons, respectively. The dispersion interaction is accounted for via the dispersion correction suggested by Grimme.[4] To reduce the computational cost, H-terminated armchair GNR with length 28.116 Å is used to simulate the graphene sheet. To avoid the interaction between two neighboring nanoribbons, a relative large supercell (16×1) with length 40.896 Å is used for the copper substrate. The copper slab consists of five-atomic layers with the bottom two layers fixed at their lattice position whereas the top three layers are allowed to relax. A portion of top-one or two layer copper atoms

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are removed to simulate the nanogrooves with two different depths. The GNR is initially located 3.04 Å above the copper surface so that the GNR only interacts with copper substrate via long-range dispersion interaction (see Fig. S1(a) and (c)). After structure optimization, the atoms from upper layer moved to the lower layer as labeled in Fig. S1(c) and (d).

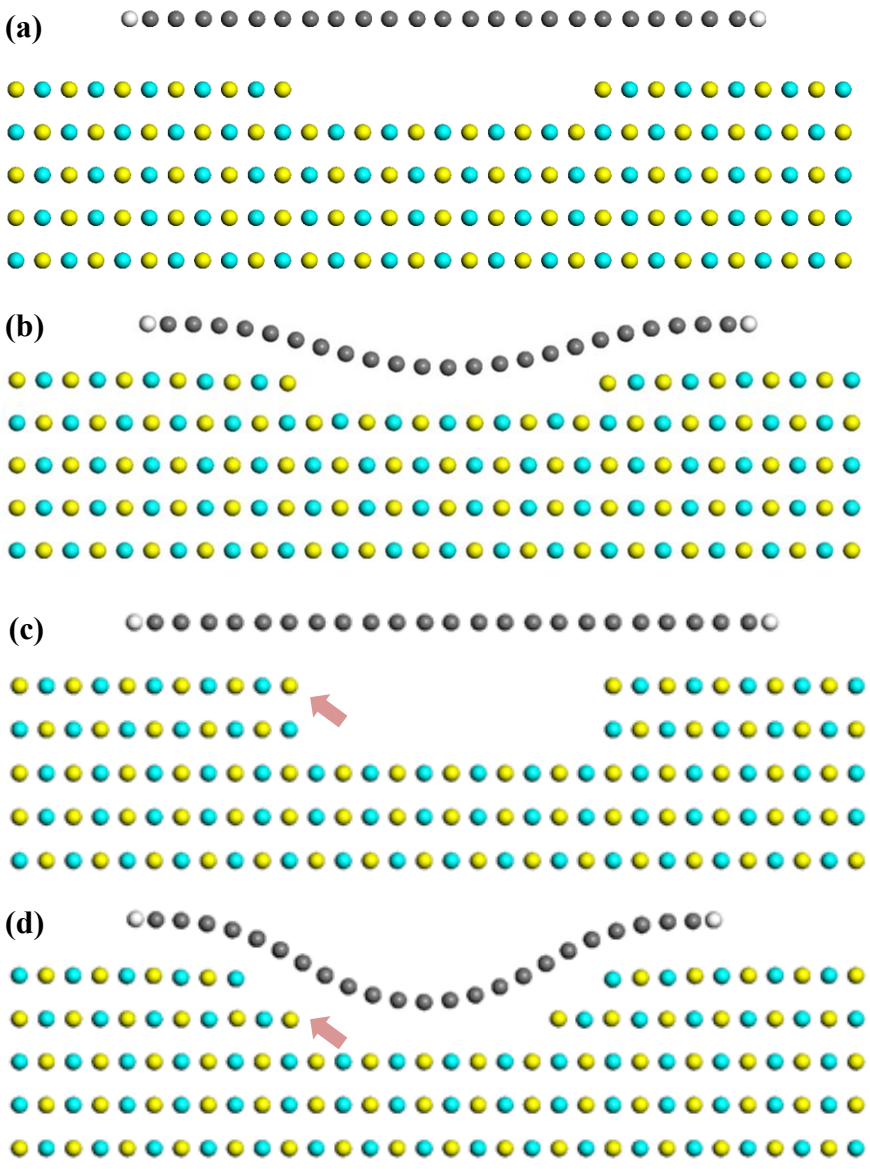

Figure S1. Optimized structures on the basis of PBE-level DFT method. (a), (b) Side view of the GNR-Cu heterostructure with nanogroove depth of 2.087 Å before and after optimization. (c), (d) Side view of the GNR-Cu heterostructure with nanogroove depth of 4.174 Å before and after optimization. The yellow and blue colors denote Cu atoms in the front and back positions, respectively.

REFERENCES

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4. S. Grimme, *J Comput Chem*, 2006, 27, 1787-1799.