

Electronic Supplementary Information

Chiral heteronanotubes: arrangement-dominated chiral interface states and conductivities

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COMPUTATIONAL DETAILS

The structural relaxations for all systems are executed by the Vienna ab initio simulation package (VASP) code with density functional theory (DFT).^{1,2} The projector-augmented wave (PAW) basis set was employed to resolve the Kohn-Sham equations.^{3,4} To guarantee the accuracy of calculations, a cutoff energy 500 eV and $1 \times 1 \times 7$ Monkhorst-Pack k -points were chosen for self-consistent calculations until the absolute force on each atom is less than 0.01 eV/Å and the electron relaxation convergence criterion was 10^{-5} eV. To avoid the interaction of the periodic images in the xy -plane, a 30×30 Å vacuum slab was built for all CHNTs. 25 k -points were set between the Γ -point and Z-point to improve the accuracy of band structure for all structures.

In quantum transport calculation, the nonequilibrium Green's function in combination with density functional theory (NEGF-DFT) implemented in NanoDcal software was employed.⁵⁻⁷ Norm-conserving pseudopotentials and linear combinations of atomic orbitals as basis sets are adopted. Double-zeta plus polarization (DZP) basis sets were utilized for all atoms and the real-space cut-off was 150 Ry and Monkhorst-Pack $1 \times 1 \times 50$ k -points which is enough to keep the accuracy for leads. The Perdew-Burker-Ernzerhof in the framework of generalized gradient approximation (GGA-PBE) exchange-correlation functional were utilized for all calculation procedures.⁸ Grimme DFT-D2 semiempirical dispersion-correction method was utilized to consider the weak van der Waals (vdW) interaction.⁹

The simulated devices consist of right/left leads, right/left buffers and scattering region. To confirm the accuracy of simulation, the parameters must be tested. The lead length does not play the most important role in transport properties. But enough K points are necessary for leads to provide all channels for calculating transport properties. If one uses longer leads, fewer K points can be set in the calculation. Buffer layers is between crystalline leads and scattering region to avoid distortions in wavefunctions under applied biases. Fully relaxed buffer layers have a good contact with scattering region. The length of buffer should be tested carefully.

Armchair chiral heteronanotubes

Fig. S2 shows the armchair and zigzag interface constructed in hexagonal atomic sheet. The polarization in BN domains is different. The polarization is parallel to BN domains in armchair interface structure, while it is vertical to BN domains in zigzag interface structure. The black arrows indicate the direction of the polarization. Fig. S3 shows the structure, band structures and chiral interface states of parallel and antiparallel armchair chiral heteronanotubes (AC-CHNTs). In comparison, the band gap of antiparallel AC-CHNT is smaller than that of parallel AC-CHNT. This is similar to zigzag chiral heteronanotubes (ZZ-CHNTs). The chiral interface states provide π channels for chiral conductivities.

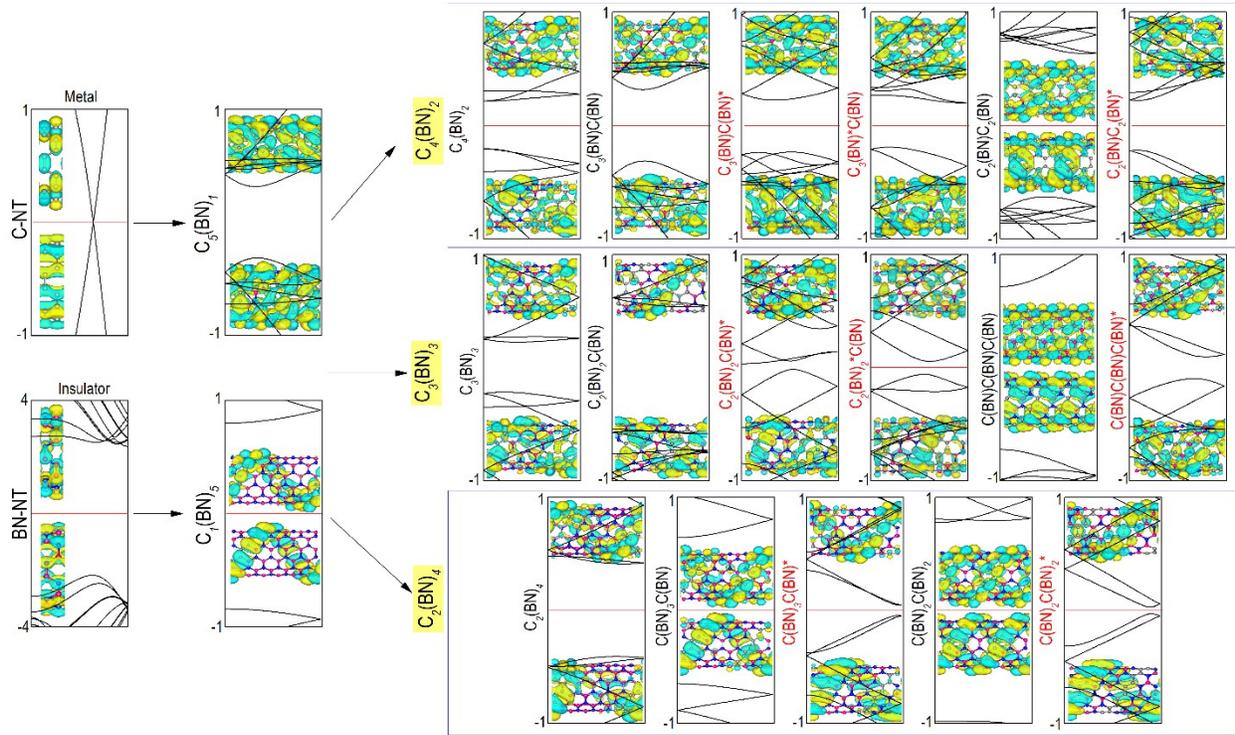


Fig. S1 Band dispersions and localized states of VBM and CBM for all CHNTs

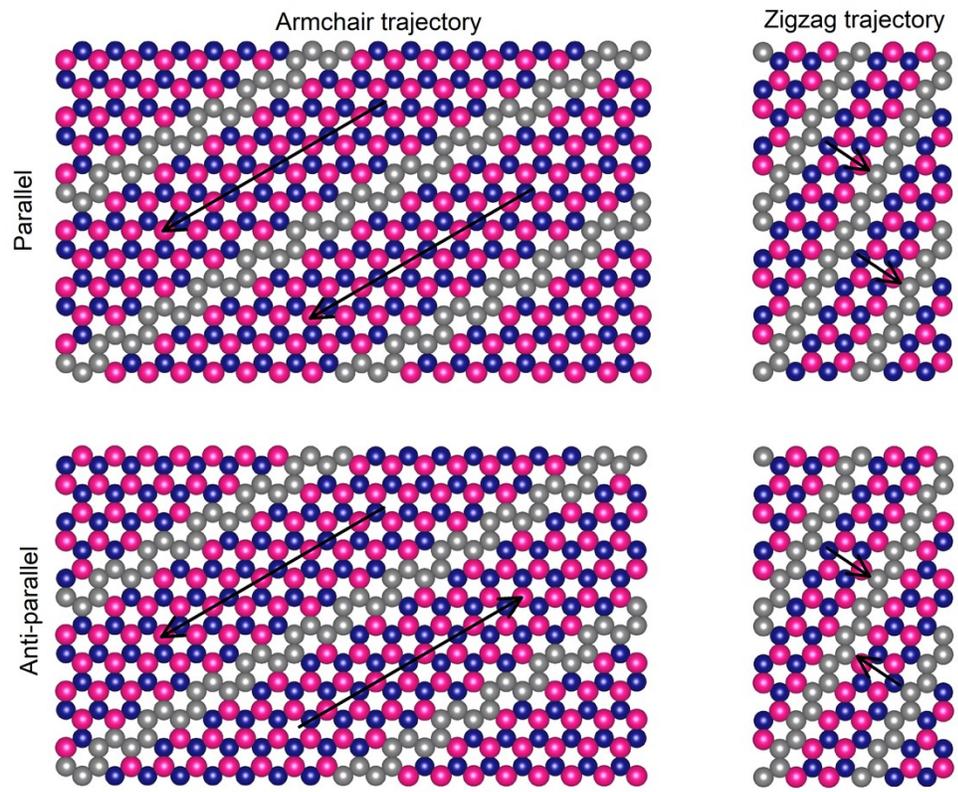


Fig. S2 Armchair and zigzag interface with parallel and antiparallel arrangements in hexagonal sheet. The black arrows indicate the direction of polarization of BN domains.

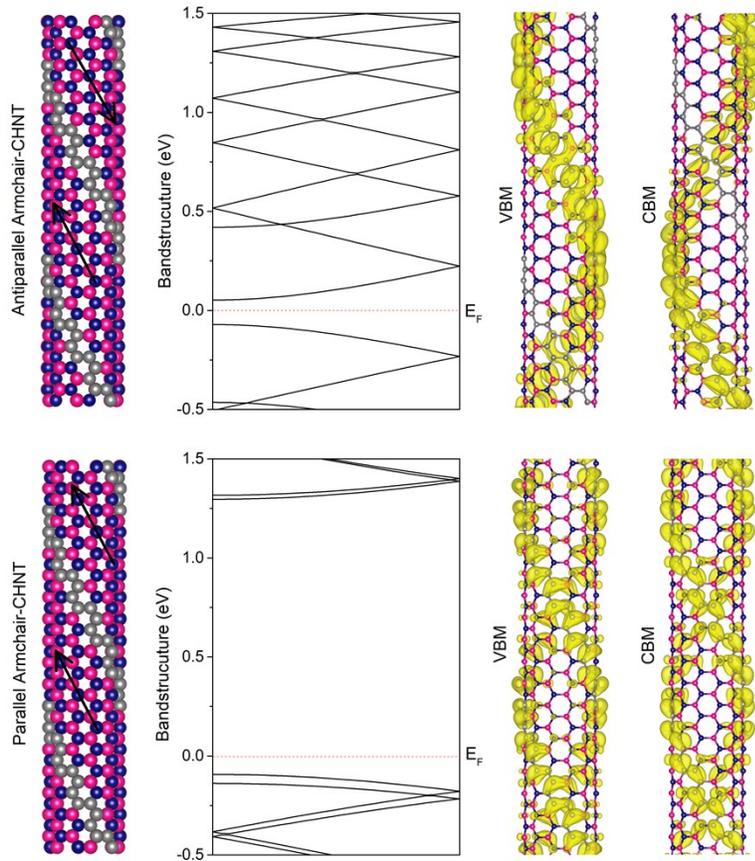


Fig. S3 Structure, band structure and chiral interface states of parallel and antiparallel armchair chiral heteronanotubes.

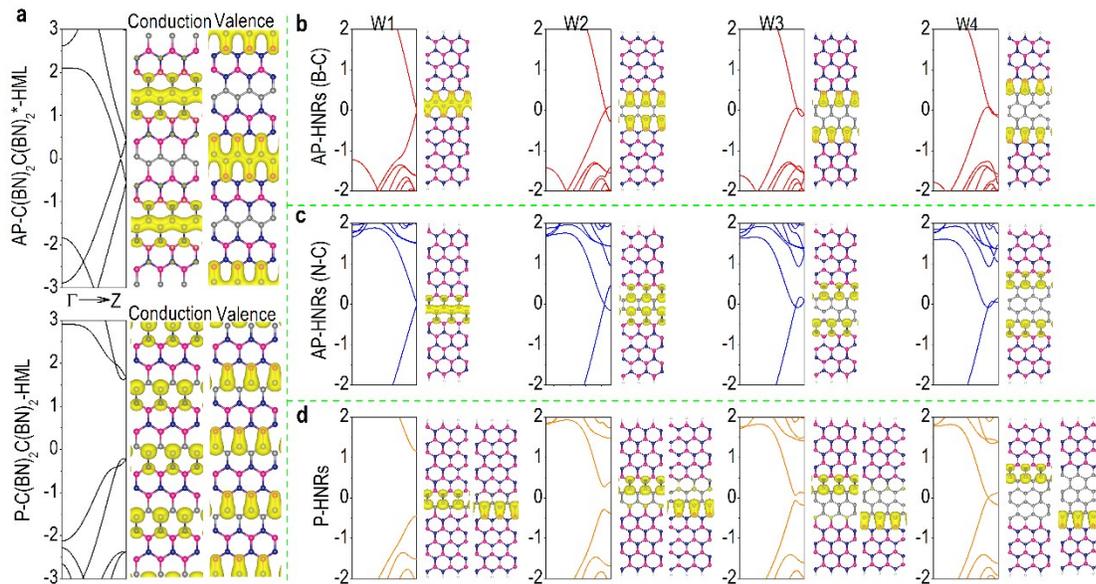


Fig. S4. Band dispersions and localized interface states of BCN HMLs and HNRs. a, Two-dimensional AP-C(BN)₂C(BN)₂* and P-C(BN)₂C(BN)₂ HML. b-d, Sandwiched h-BN/graphene/h-BN HNRs, including AP-HNRs with double C-B interfaces (b), AP-HNRs with double N-C interfaces (c) and P-HNRs with both of B-C and N-C interface (d).

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