Supplementary Material for

Electronic structure and transport properties of 2D RhTeCl: A NEGF-DFT study

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Fig. S1. Side view of optimized bulk RhTeCl along b and a directions. L and d_0 represent the thickness of each layer and the van der Waals gap, respectively.

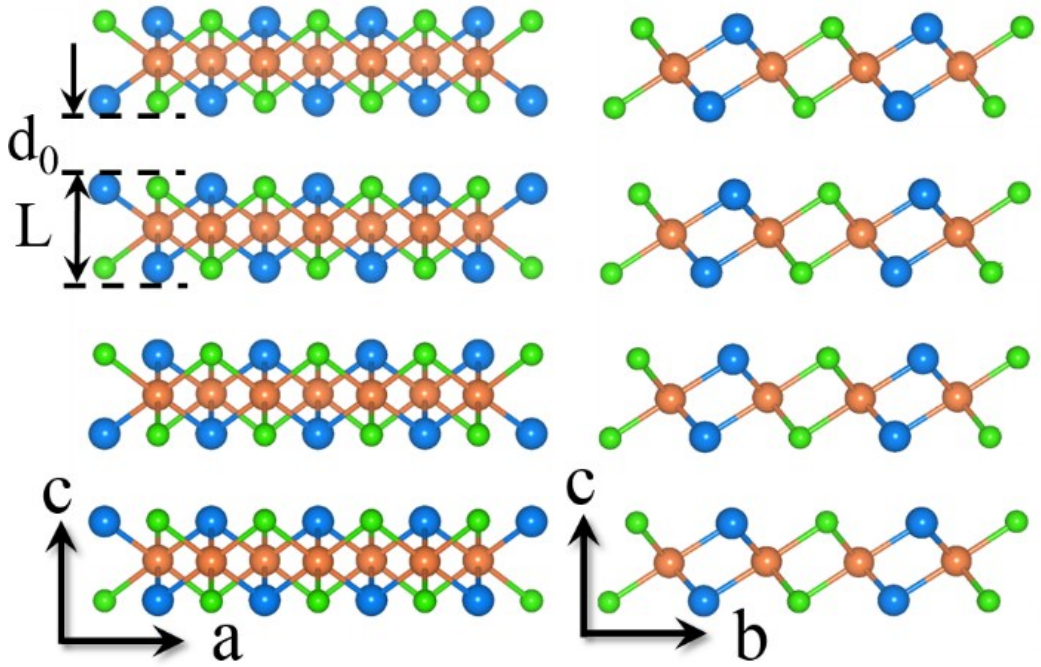
Fig. S2. Top and side views of snapshot for 5×4×1 monolayer RhTeCl at 10 ps of the molecular dynamics simulations.

Fig. S3. The electronic band structure of bulk RhTeCl at PBE level.

Fig. S4. Electronic band structures of monolayer RhTeCl calculated in the basic of (a) PBE and (b) HSE06 when considering with SOC.

Fig. S5. (a) Strain-total energy relations and the energy shifts of (b) CBM and (c) CBM with respect the vacuum energy under uniaxial strain along the a and b directions for RhTeCl monolayer (Δl refers to the dilation along a or b, whereas l_0 refers to the lattice constant of a or b at equilibrium geometry).

Fig. S6 Change of the LDOS and the spectral current under a V_{gs} variation of 0.2 V in the double-gate monolayer RhTeCl n-MOSFET with L_g = 6 nm.



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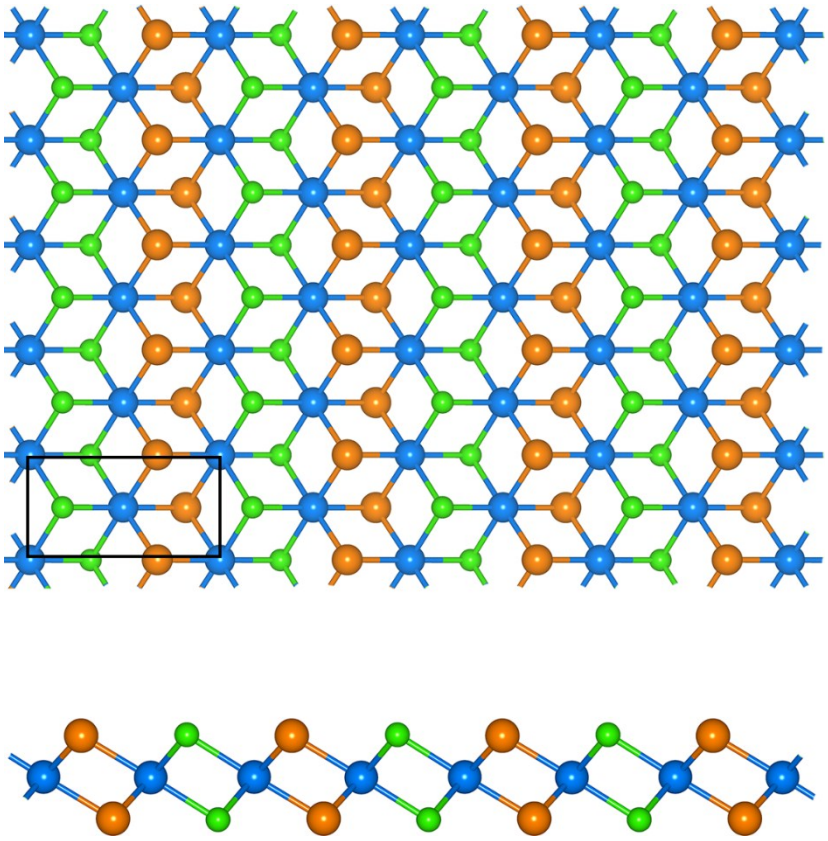

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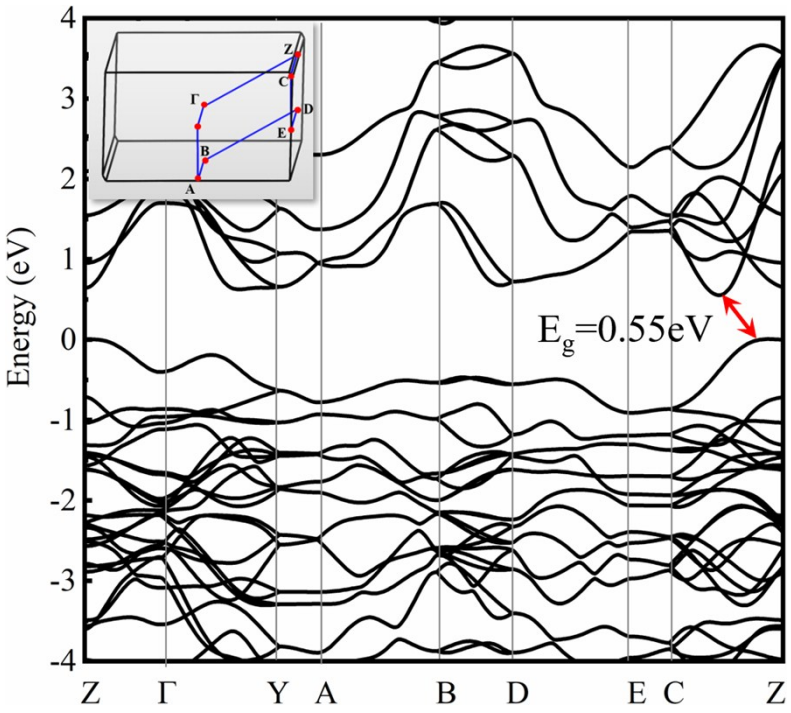

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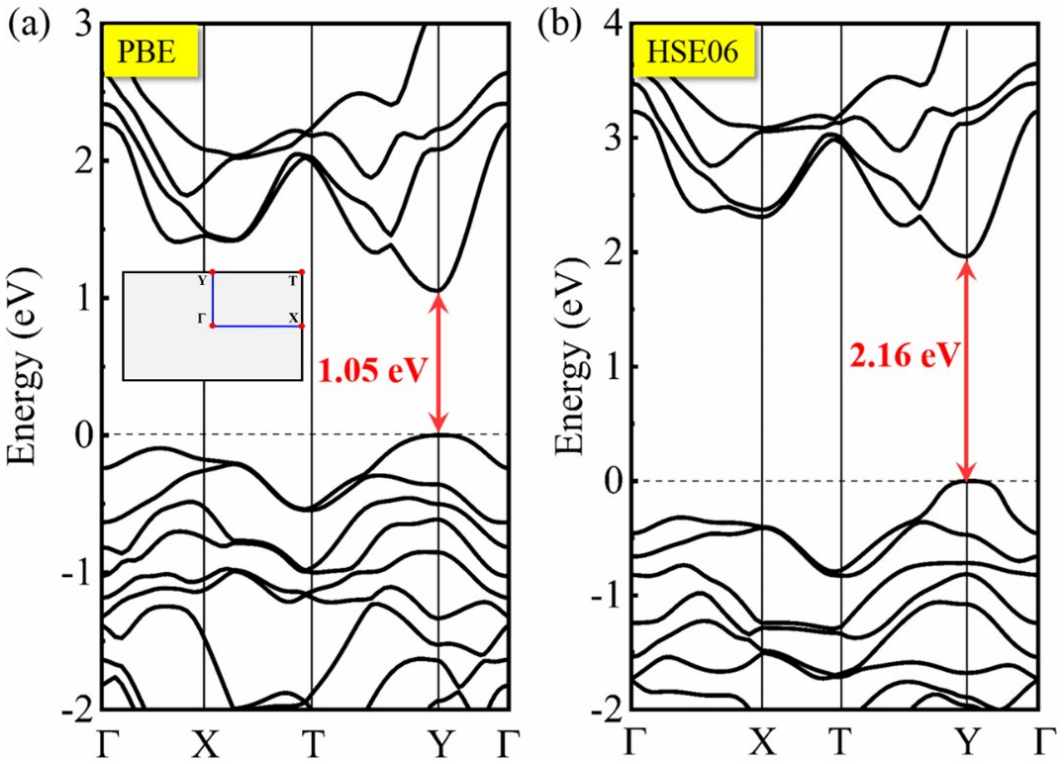

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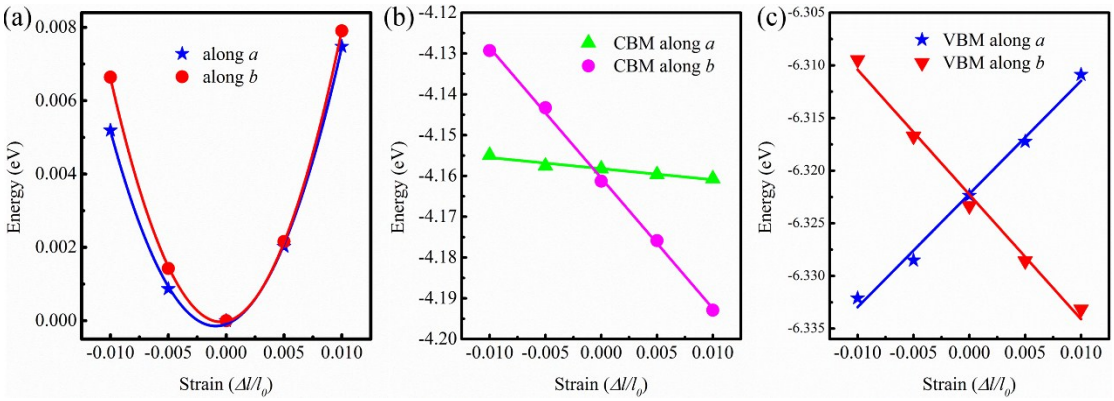

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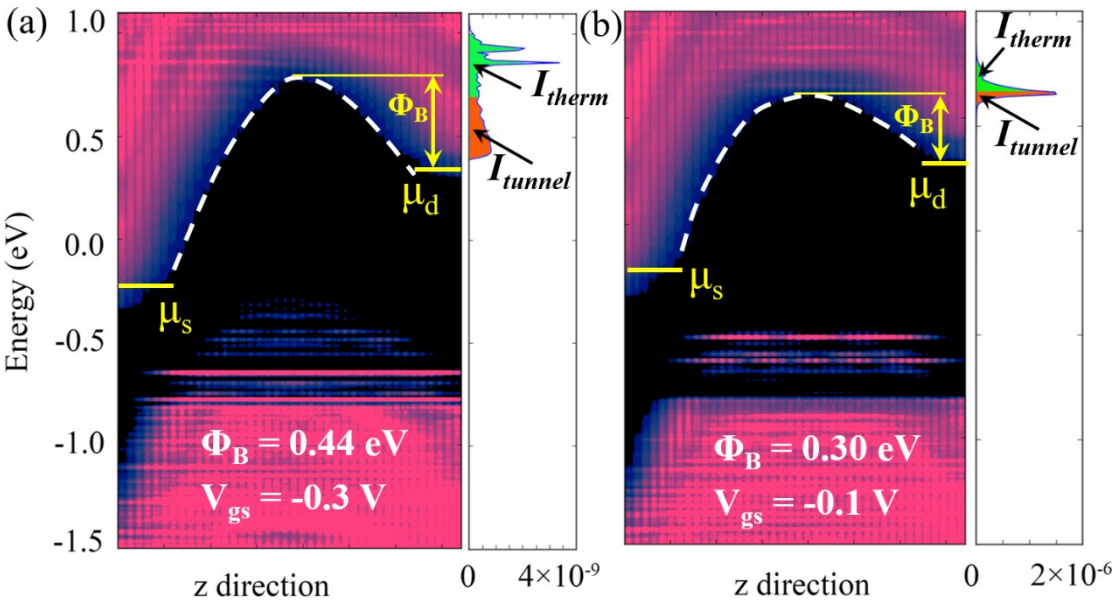

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