Supporting Information: DFT coupled with NEGF study of a promising two-dimensional channel material: Black phosphorene-type GaTeCl

Wenhan Zhou,[a] Shiying Guo,[a] Shengli Zhang,[a,*] Zhen Zhu,[b] Xiufeng Song,[a] Tianchao Niu,[a] Kan Zhang,[a] Xuhai Liu,[a] Yousheng Zou,[a] Haibo Zeng[a,*]

[1]Key Laboratory of Advanced Display Materials and Devices, Ministry of Industry and Information Technology, College of Material Science and Engineering, Nanjing University of Science and Technology, Nanjing 210094, China

[2]Materials Department, University of California, Santa Barbara, CA 93106, USA

**Corresponding author: zhangslvip@njust.edu.cn and zeng.haibo@njust.edu.cn*

TABLE SI. Structural information for few-layers GaTeCl. (Lattice constants a (Å), b (Å), L_1 (Å) and L_2 (Å) of few-layers GaTeCl.)

Models	a (Å)	b (Å)	L_1 (Å)	L_2 (Å)
1L	4.090	5.796	5.22	
2L	4.085	5.833	5.14	2.09
3L	4.083	5.841	5.13	2.09
4L	4.081	5.845	5.13	2.10
5L	4.080	5.848	5.13	2.10
6L	4.080	5.848	5.13	2.10
Bulk	4.080	5.853	5.08	2.10

TABLE SII. The calculated effective mass (m*) and mobility (μ) of electrons and holes along Γ-X and Γ-Y directions for monolayer GaTeCl at 300 K.

Carrier type	**m* x/m_0**	**m* y/m_0**	**E_{lx} (eV)**	**E_{ly} (eV)**	**C_{x_2D} (J m^{-2})**	**C_{y_2D} (J m^{-2})**	**μ_{x_2D} ($cm^2V^{-1}s^{-1}$)**	**μ_{y_2D} ($cm^2V^{-1}s^{-1}$)**
e^-		0.61		3.16	52.64	28.98		109.56
h^+	0.16	0.69	2.65	3.58	52.64	28.98	4.71×10^3	66.72

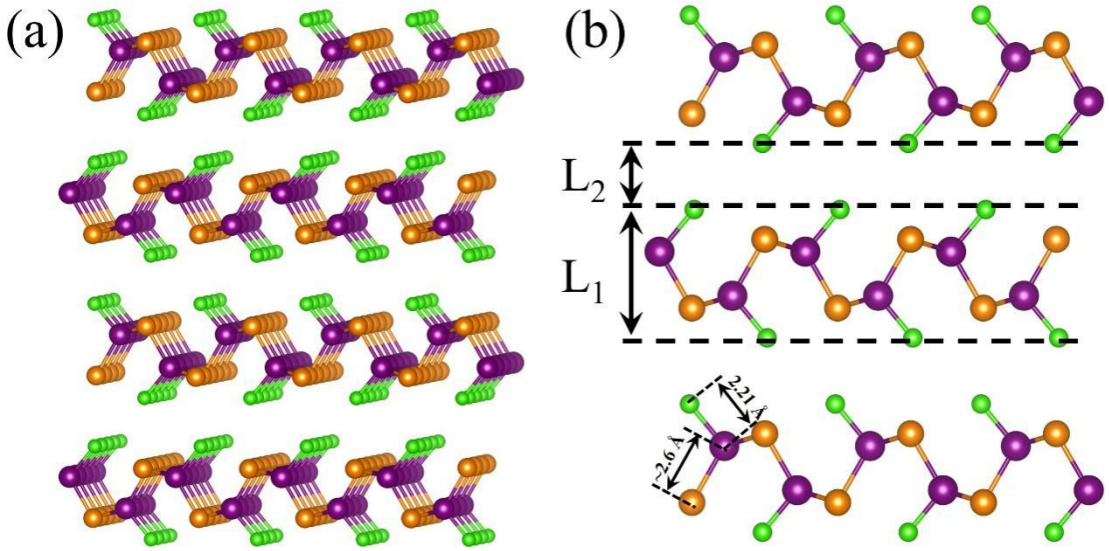

Figure S1. (a) Crystal structure of bulk GaTeCl. (b) schematic diagram of few-layers GaTeCl.

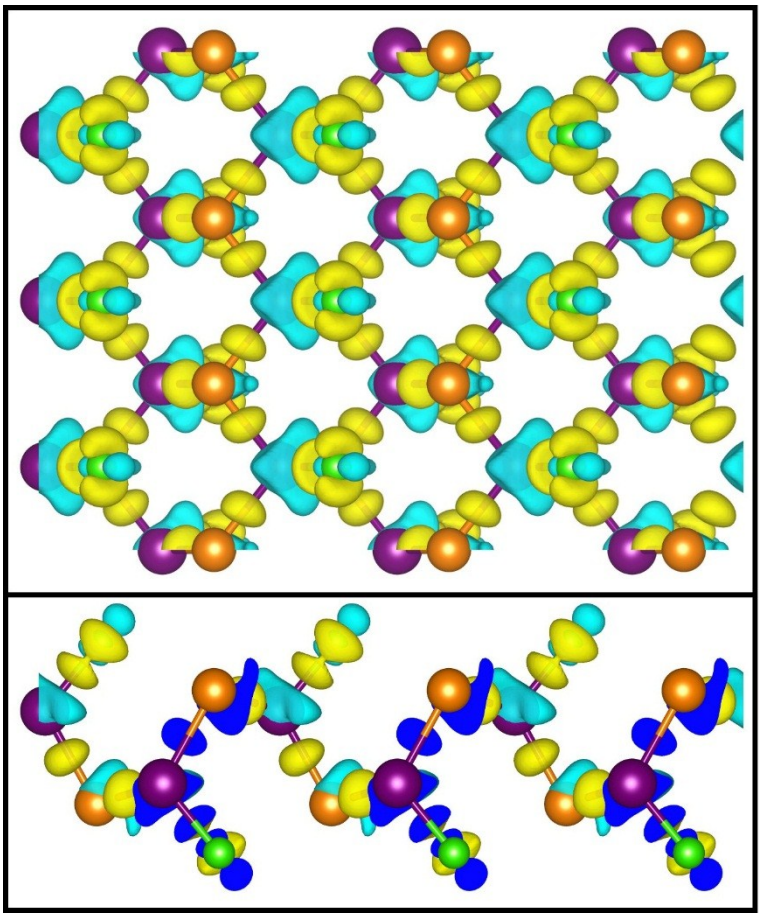

Figure S2. Deformation charge density of monolayer GaTeCl. Yellow and cyan refer to electron accumulation and depletion regions, respectively.

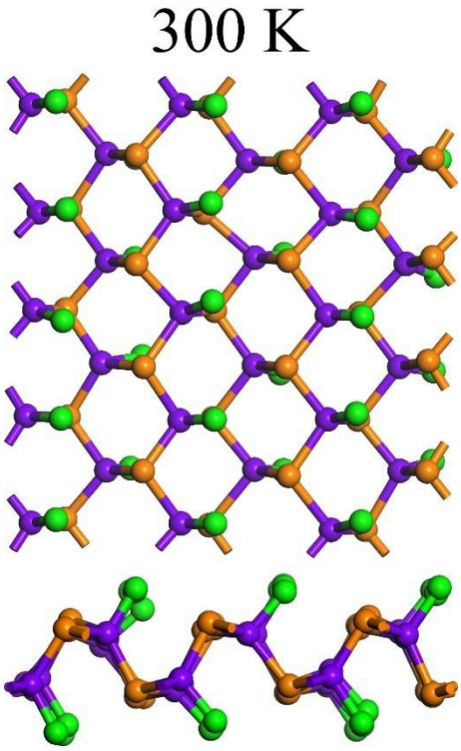

Figure S3. selected snapshots of monolayer GaTeCl structure in MD simulations at 300 K.

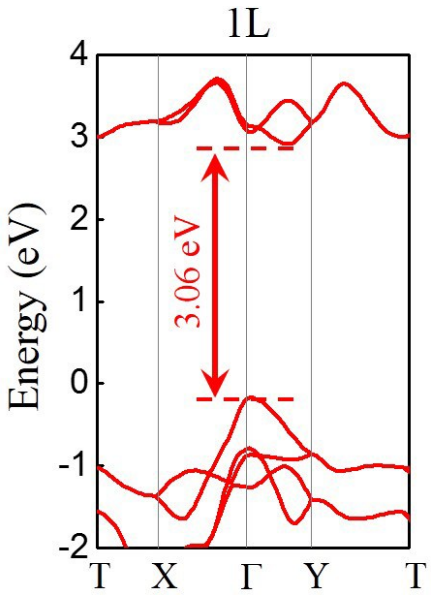

Figure S4. The electronic band structure of monolayer GaTeCl based on HSE06.

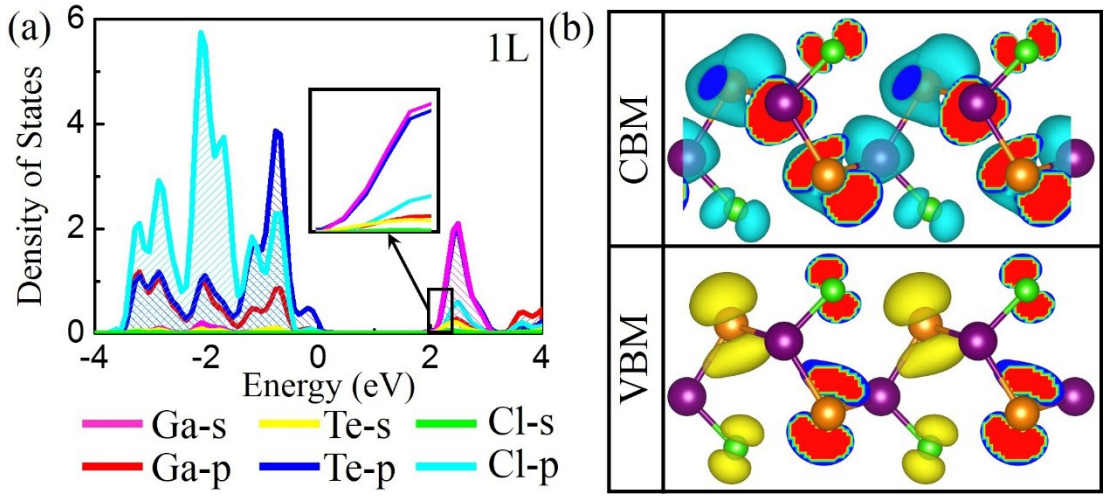

Figure S5. (a) The PDOS of GaTeCl monolayer. (b) The iso-surfaces of partial charge densities for the VBM and CBM of GaTeCl monolayer.

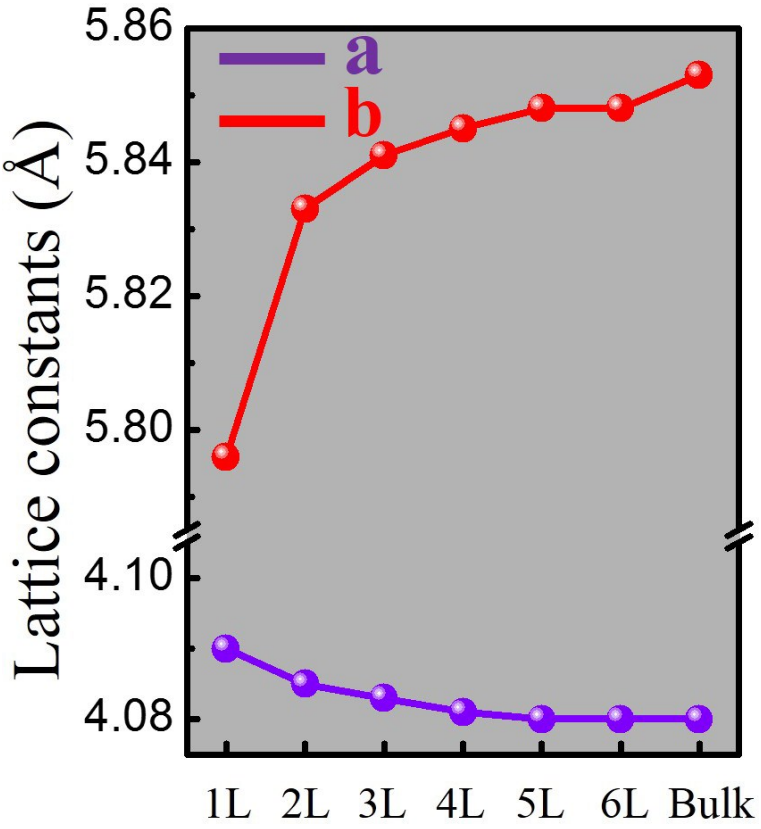

Figure S6. Variation of the lattice constants **a** and **b** with layer number for GaTeCl.

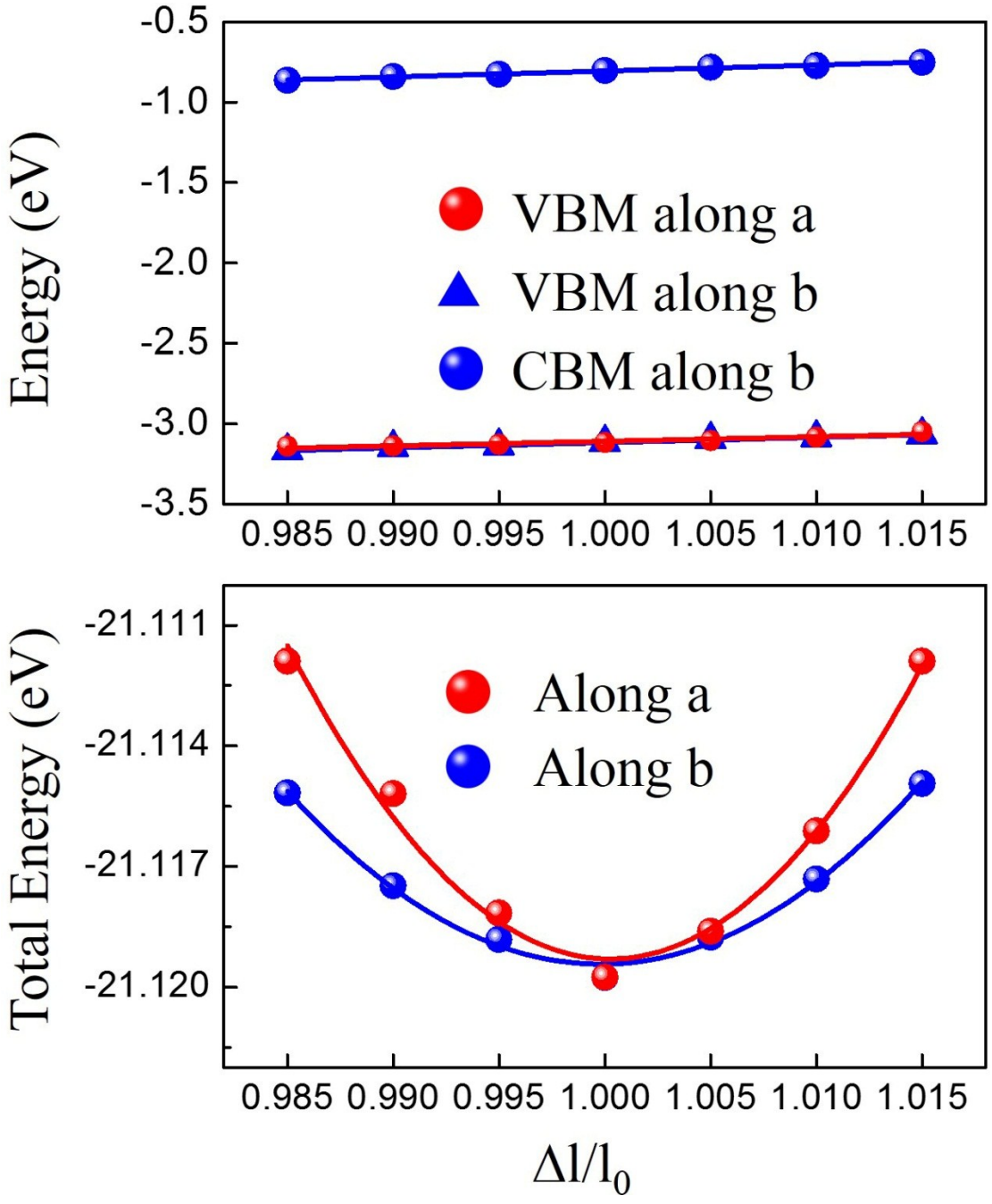

Figure S7. (a) Shifts of VBM and CBM and (b) strain-total energy relations under uniaxial strain along a and b directions for GaTeCl monolayer sheet, Δl refers to the dilation along a or b, while l_0 refers to the lattice constant of a or b at equilibrium geometry. In (a), the vacuum level is set at zero for reference.

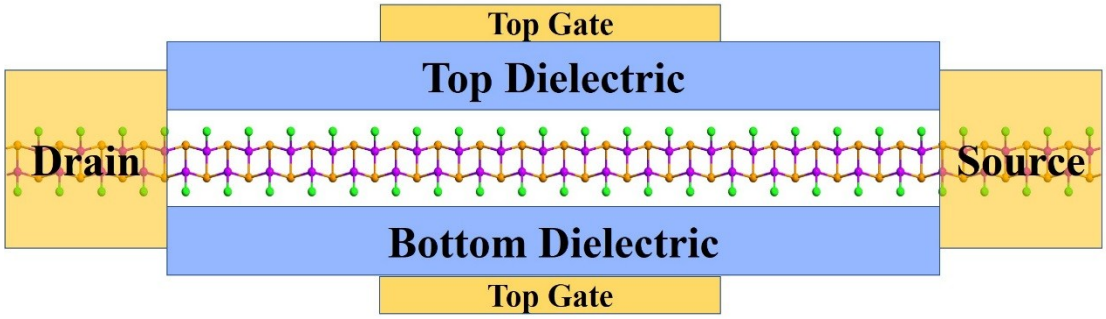

Figure S8. Schematic of GaTeCl double-gated MOSFET with symmetric UL structures.