

Supporting Information

In-plane CrI₂/CrI₃ 2D superlattice: novel electronic properties and strain induced phase transition

Yuanyuan Zhao¹, Hongsheng Liu^{1,2*}, Jijun Zhao¹, Junfeng Gao^{1,2*}

1 Key Laboratory of Materials Modification by Laser, Ion and Electron Beams (Dalian University of Technology), Ministry of Education, Dalian 116024, China

2 Dalian University of Technology and Belarusian State University Joint Institute & Innovation Center, Dalian 116024, China

Corresponding authors: liuhongsheng@dlut.edu.cn, gaojf@dlut.edu.cn

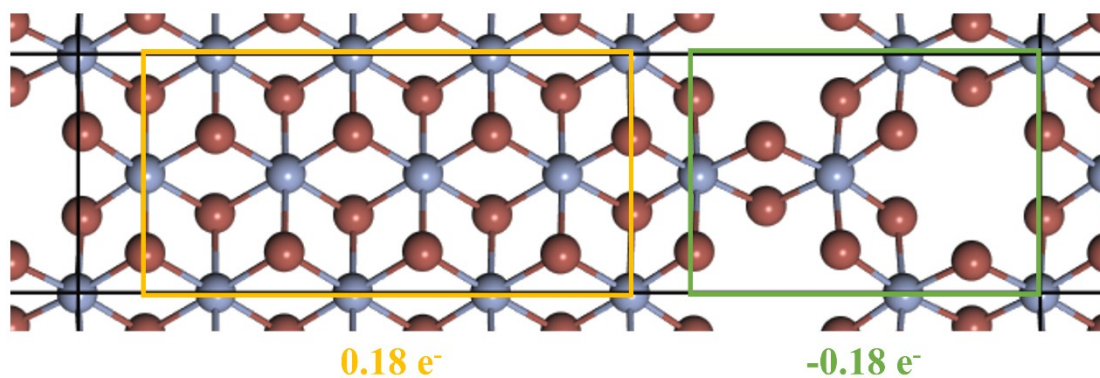


Figure S1. Bader charge transfer in CrI₂(4)/CrI₃(1) superlattice. Areas in the orange and green rectangles are CrI₂ and CrI₃ parts, respectively. Negative value means the gain of electrons and positive value means loss of electrons. Accordingly, 0.18 electron transfers from the CrI₂ part to the CrI₃ part.

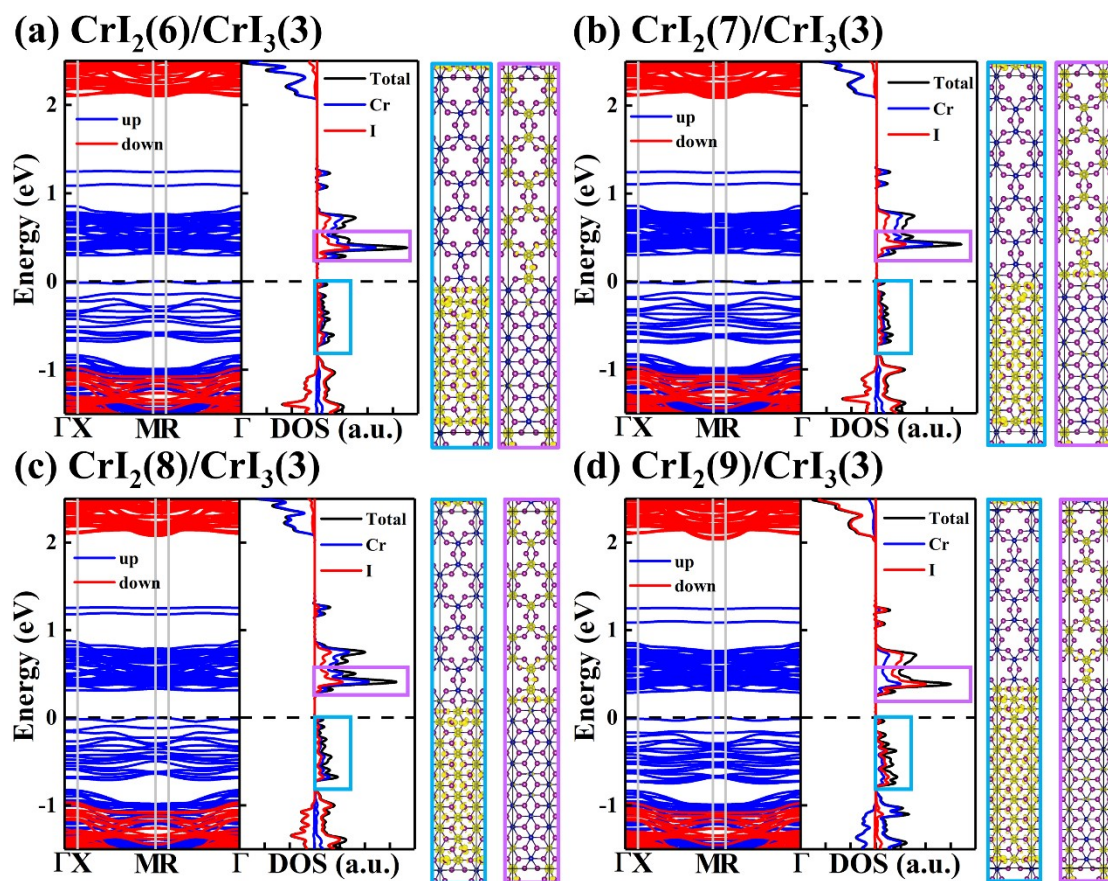


Figure S2. Electronic band structures, projected density of states and band decomposed charge densities of (a) $\text{CrI}_2(6)/\text{CrI}_3(3)$, (b) $\text{CrI}_2(7)/\text{CrI}_3(3)$, (c) $\text{CrI}_2(8)/\text{CrI}_3(3)$, (d) $\text{CrI}_2(9)/\text{CrI}_3(3)$. The Fermi level is scaled to zero. The charge density in blue and purple rectangles are from the bands indicated by blue and purple rectangles in the PDOS, respectively. The charge density isosurface is $0.005 \text{ e}/\text{\AA}^3$.

CrI₂(11)/CrI₃(3)

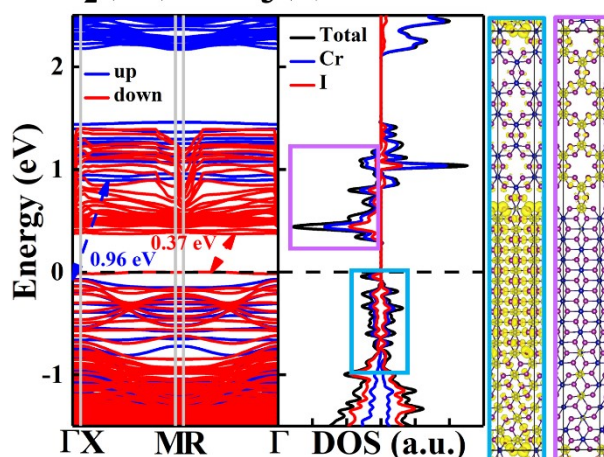
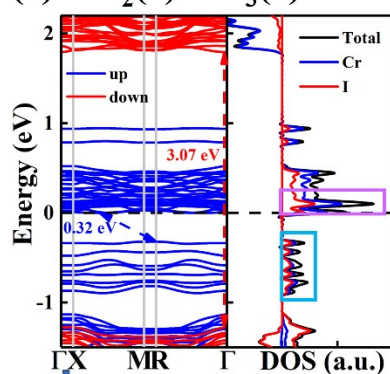


Figure S3. Electronic band structures, projected density of states and band decomposed charge densities of CrI₂(11)/CrI₃(3). The Fermi level is scaled to zero. The charge density in blue and purple rectangles are from the bands indicated by blue and purple rectangles in the PDOS, respectively. The charge density isosurface is 0.005 e/Å³.

(a) CrI₂(4)/CrI₃(2)



(b) CrI₂(4)/CrI₃(4)

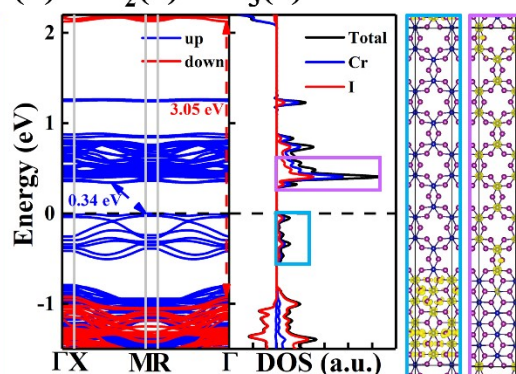


Figure S4. Electronic band structures, projected density of states and band decomposed charge densities of (a) CrI₂(4)/CrI₃(2), (b) CrI₂(4)/CrI₃(4). The Fermi level is scaled to zero. The charge density in blue and purple rectangles are from the bands indicated by blue and purple rectangles in the PDOS, respectively. The charge density isosurface is 0.005 e/Å³.

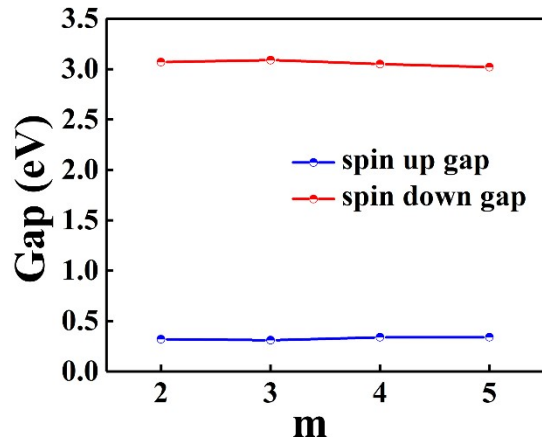


Figure S5. Band gap as a function of the width of CrI₃ ribbon in CrI₂(4)/CrI₃(m) superlattices.

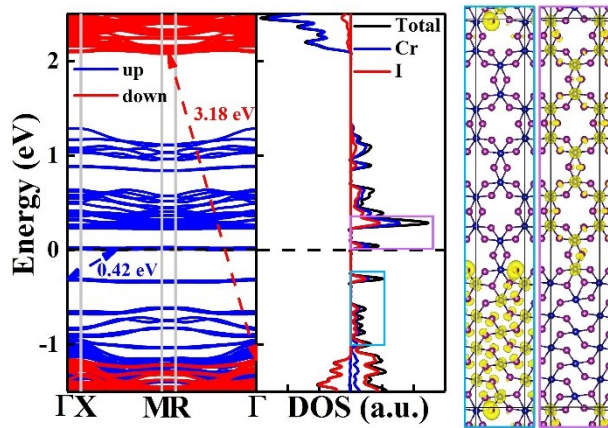


Figure S6. Electronic band structure, projected density of states and band decomposed charge densities of CrI₂(4)/CrI₃(3) superlattice under tensile strain of 6%. The Fermi level is set to zero. The charge density in blue and purple rectangles are from the bands indicated by blue and purple rectangles in the PDOS, respectively. The charge density isosurface is 0.005 e/Å³.