Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information: Achieving Direct Band Gap and High Power Conversion Efficiency in SbI_3/BiI_3 Type-II vdW Heterostructure via Interlayer Compression and Electric Field

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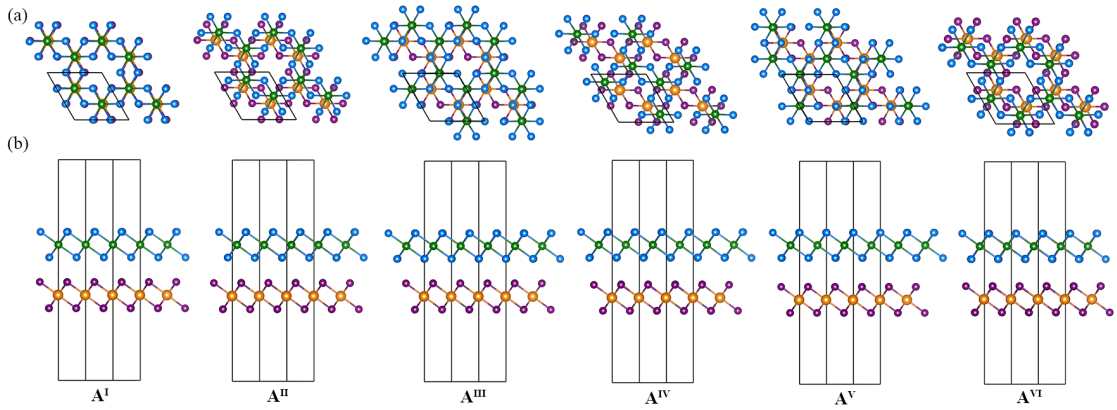

Figure S1: Top (a) and side (b) view of six selected configurations within SbI_3/BiI_3 moiré pattern A. The green, yellow, blue and purple balls represent Sb, Bi, and I atoms, respectively.

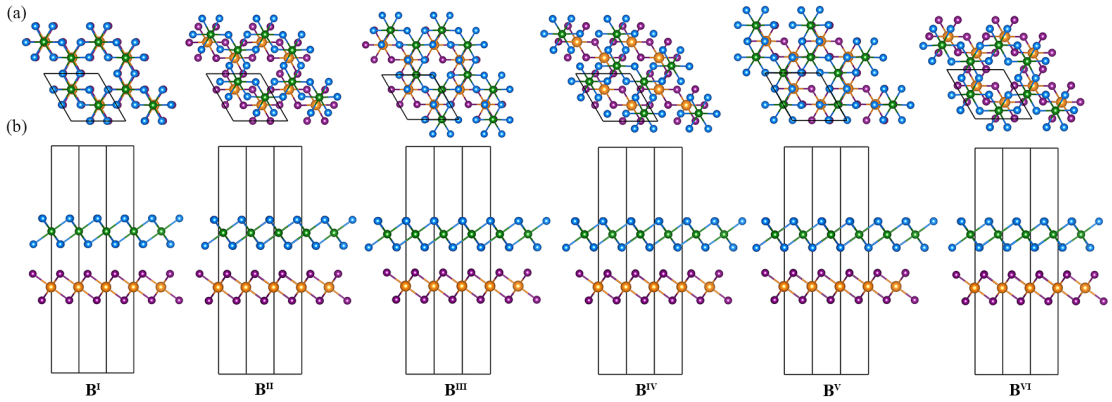

Figure S2: Top (a) and side (b) view of six selected configurations within SbI_3/BiI_3 moiré pattern B. The green, yellow, blue and purple balls represent Sb, Bi, and I atoms, respectively.

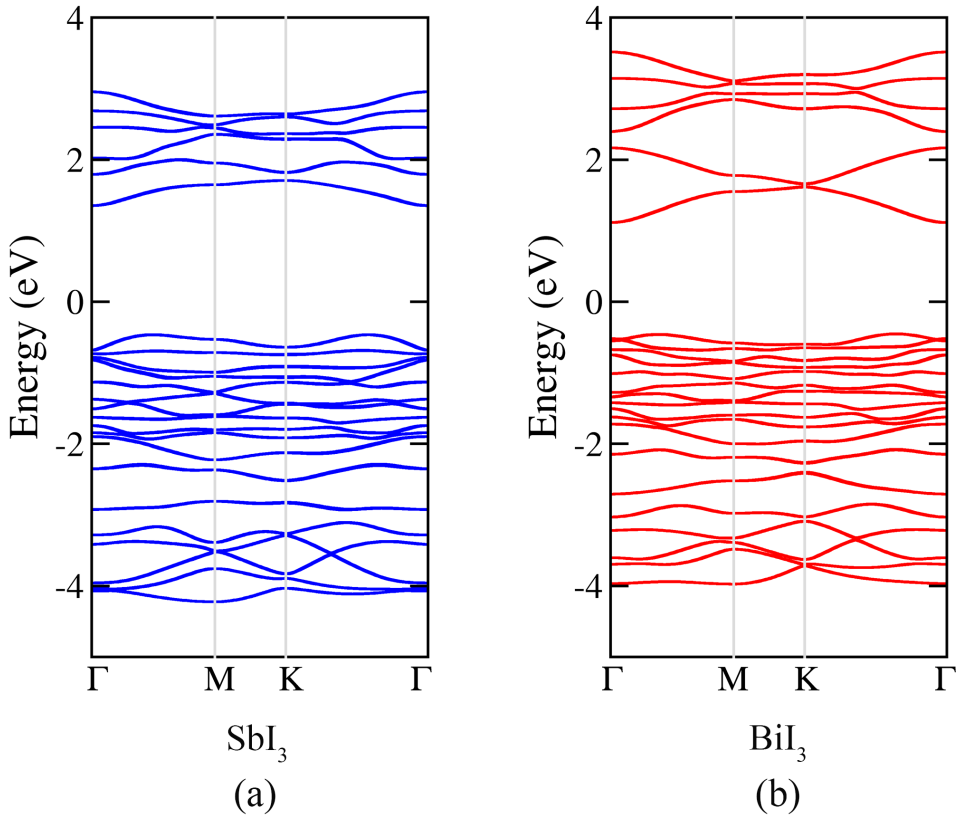

Figure S3: The electronic band structure of free-standing BiI_3 and stretched SbI_3 single-layer.

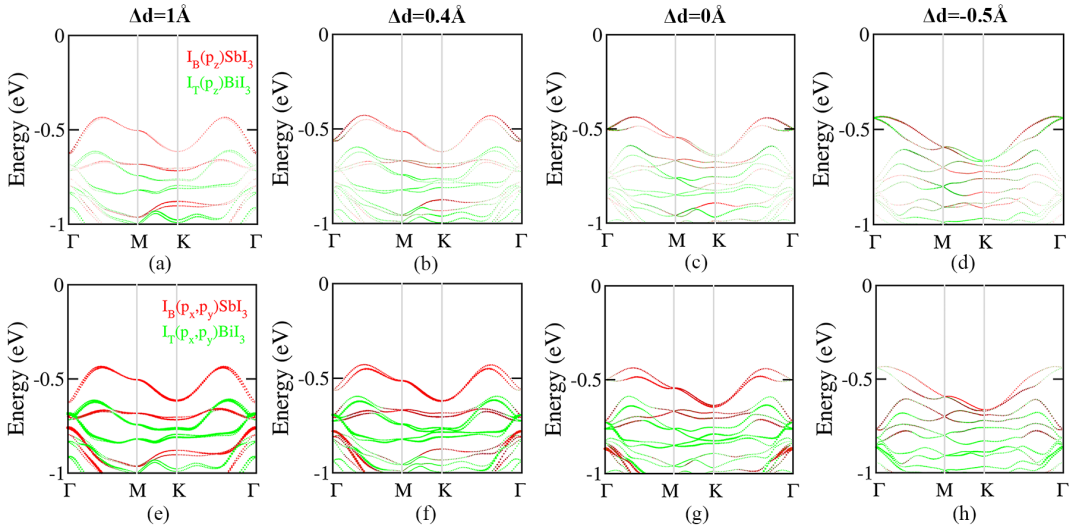

Figure S4: The orbitals-projected band structure of interlayer I(p_z) states ((a)-(d)) and I(p_x,p_y) states ((e)-(h)) with different interlayer distances.

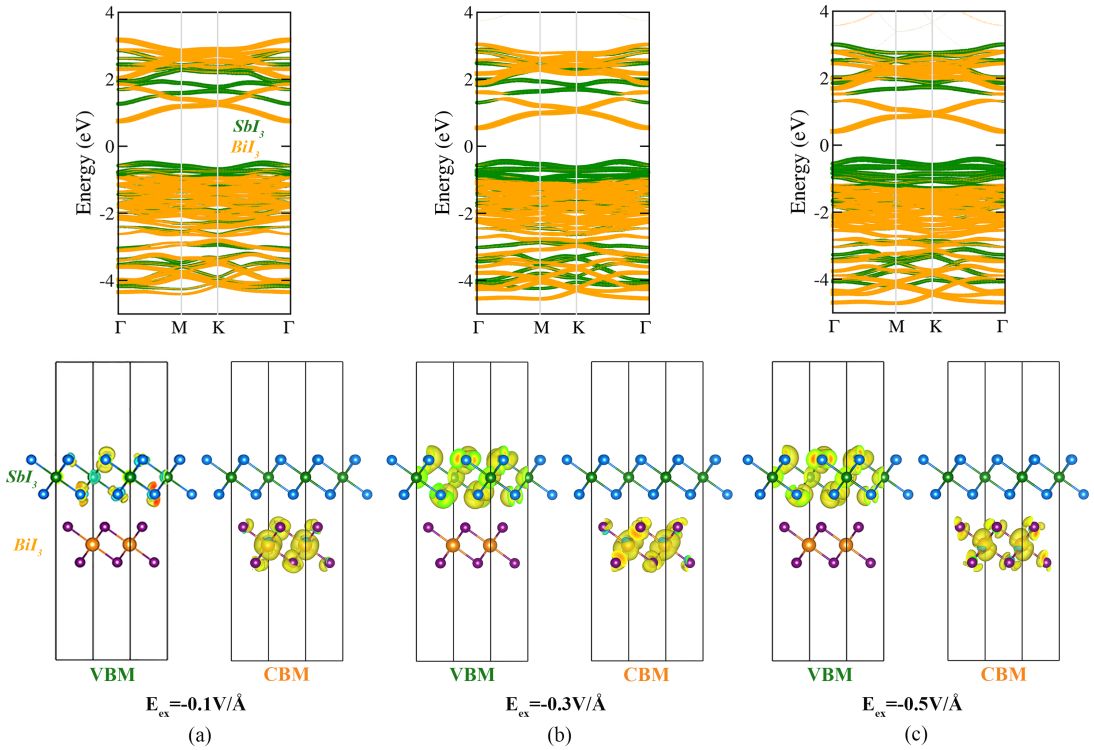

Figure S5: The layer-projected band structure and the isosurface of charge density of the VBM and CBM of SbI_3/BiI_3 vdW heterostructure under -0.1(a), -0.3(b) and -0.5V/Å(c) electric field. The value of isosurface is 0.00055 e/bohr^3.

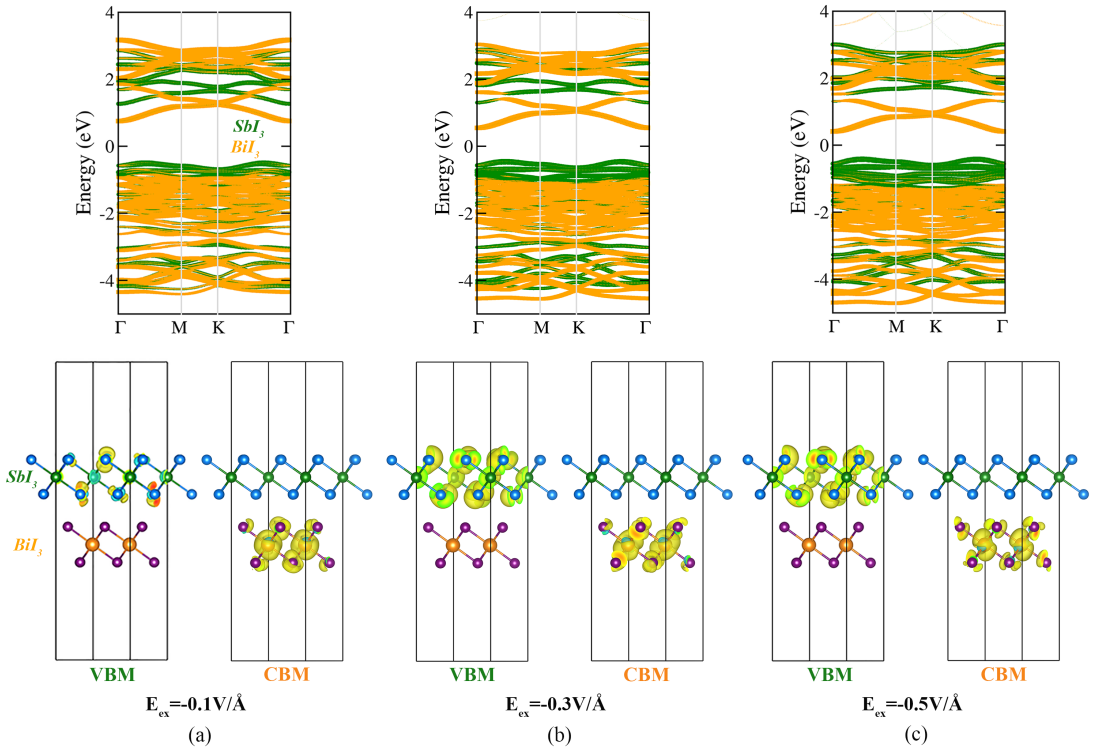

Figure S6: The layer-projected band structure and the isosurface of charge density of the VBM and CBM of SbI_3/BiI_3 vdW heterostructure under 0.1(a), 0.3(b) and 0.5V/Å(c) electric field. The value of isosurface is 0.00055 e/bohr^3.