Supporting Information

Ultra-flexible two-dimensional Janus heterostructure superlattice: A novel intrinsic wrinkled structure

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The first-principles calculations were based on density functional theory (DFT), using Vienna *ab initio* simulation package (VASP).[1, 2] The projector augmented wave potentials (PAW) were conducted to describe the core electrons[3] with the generalized gradient approximation (GGA).[4] The Perdew–Burke–Ernzerhof (PBE) functional was also used to describe the exchange correlation functional. The cut-off energy is 500 eV and a 17 × 17 × 1 Monkhorst–Pack *k*-point grids were considered in the first Brillouin zone. The convergence for force and energy are set as 0.01 eV·Å^{-1} and 0.01 meV, respectively. The stress-strain results of the AA MoSSe/WSSe heterostructure by first-principles calculations are presented in Fig. S1.

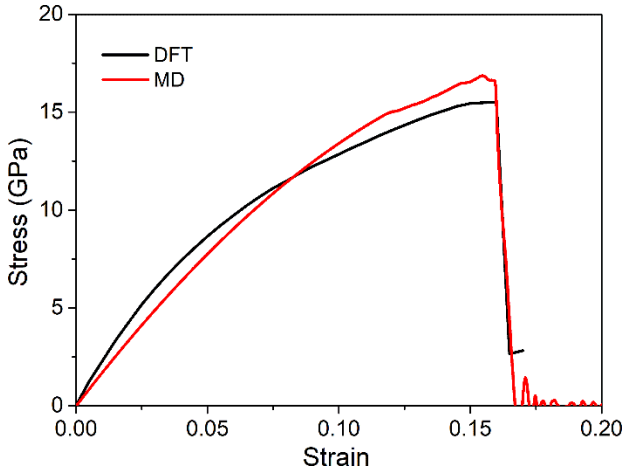

Fig. S1 The stress-strain curves of the AA MoSSe/WSSe heterostructure superlattice calculated by DFT and MD methods at 10 K.

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2. G. Kresse and J. Furthmüller, *Comp. Mater. Sci*, 1996, **6**, 15–50.

3. G. Kresse and J. Furthmüller, *Phys. Rev. B*, 1996, **54**, 11169.

4. J. P. Perdew, K. Burke and M. Ernzerhof, *Phys Rev Lett*, 1996, **77**, 3865.