## **Supplementary Materials**

## 2H→1T' Phase Transformation in Janus Monolayer MoSSe and MoSTe: an Efficient Hole Injection Contact for 2H-MoS<sub>2</sub>

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**Figure S1** A 2×1 rectangular supercell used for calculation of elastic constants and in-plane stiffness,  $a_x$  and  $a_y$  are the lattice constants of the unit cell in *x*- and *y*-directions, respectively. The elastic strain directions of  $\varepsilon_x$  and  $\varepsilon_y$  are indicated by red arrow. Bottom shows the three-dimensional fitted surface plots of strain energy versus elastic strain for the 2H- and 1T'-MoSX monolayer.

**Figure S2** The band structures of 2H- and 1T'-MoS<sub>2</sub>, which are orbitally resolved into dxy, dxz, dyz,  $dz^2$ ,  $dx^2$ - $y^2$ , and S *p* orbitals.

**Figure S3** The band structures of 2H- and 1T'-MoSTe, which are orbitally resolved into dxy, dxz, dyz,  $dz^2$ ,  $dx^2$ - $y^2$ , S *p* and Te *p* orbitals.



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**Figure S3** The band structures of 2H- and 1T'-MoSTe, which are orbitally resolved into dxy, dxz, dyz,  $dz^2$ ,  $dx^2$ - $y^2$ , S p and Te p orbitals.