Supporting information for

## Pseudo Janus Based on Rhombohedral Homobilayer Transition Metal Dichalcogenides

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E-mail: <u>xubo@cpu.edu.cn;</u> putaochen@njtech.edu.cn; <u>iamyccheng@njtech.edu.cn</u> **Keywords:** rhombohedral bilayer, electric polarization, piezoelectricity, spin-dipole locking effect, Rashba splitting



Figure S1. The structure and simulated HRTEM images for 2H and two 3R stacking tri-layer MoS<sub>2</sub>. (a) Side view and (b) top view of three stacking trilayer MoS<sub>2</sub>. (c) Simulated HRTEM of three tri-layer MoS<sub>2</sub> from top view.



Figure S2. Layer and spin projected band structure of tri-layer MoS<sub>2</sub>. (a-c) Lower, middle, and upper layer projected band structure of tri-layer MoS<sub>2</sub>. (d) Spin sz projected band structure of tri-layer MoS<sub>2</sub>. (e) Scheme of valence band and conduction band edges around K point for tri-layer MoS<sub>2</sub>. (f) Layer and spin projected states for tri-layer MoS<sub>2</sub>.



Figure S3. Rashba splitting of (a) tri-layer, (b) quadra-layer and (c) bulk 3R MoTe<sub>2</sub>.