Large perpendicular magnetic anisotropy of transition metal dimers driven by polarization switching of two-dimensional ferroelectric In$_2$Se$_3$ substrate

Wen Qiao, a Deyou Jin, a Wenbo Mi, b Dunhui Wang, a Shiming Yan, *a Xiaoyong Xu, *c Tiejun Zhou a

a School of Electronics and Information, Hangzhou Dianzi University, Hangzhou 310018, China

b Tianjin Key Laboratory of Low Dimensional Materials Physics and Preparation Technology, School of Science, Tianjin University, Tianjin 300354, China

c School of Physics Science and Technology, Yangzhou University, Yangzhou, 225002, China
Fig. S1 Charge difference between the total charge density and the sum of charge densities of a suspended transition metal dimers and In$_2$Se$_3$ for (a) In$_2$Se$_3$-CoCo, (b) In$_2$Se$_3$-CoOs, (c) In$_2$Se$_3$-OsCo and (d) In$_2$Se$_3$-OsOs.

Fig. S2 Dependence of size of supercell on the MAE of Os atom in In$_2$Se$_3$-CoOs with FE polarization P↓. Inset show the charge difference density of the 3×3 In$_2$Se$_3$-CoOs supercell with FE polarization P↓.
Fig. S3 PDOS of Co atom and Os atom in In$_2$Se$_3$-Co and In$_2$Se$_3$-Os with FE polarization P↑ and P↓.

Fig. S4 Orbital-resolved MAE of Co atom in In$_2$Se$_3$-Co with FE polarization P↑ and P↓.
Fig. S5 $d_{z^2}$ PDOS of (a) Co1 and Co2 atoms in In$_2$Se$_3$-CoCo, (b) Co and Co atoms in In$_2$Se$_3$-CoOs and (c) Co atom in In$_2$Se$_3$-Co with FE polarization $P\uparrow$ and $P\downarrow$. 