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Voltage-Controllable Colossal Magnetocrystalline Anisotropy in Single Layer Dichalcogenides[1] XUELEI SUI, Tsinghua University, TAO HU, California State University Northridge, JIANFENG WANG, Computational Science Research Center, Beijing, BING-LIN GU, WENHUI DUAN, Tsinghua University, MAO-SHENG MIAO, California State University Northridge — Materials with large magnetocrystalline anisotropy and strong electric field effects are in great need for new types of memory devices that are based on electric field control of spin orientations. Instead of using modified transition metal films, we propose that some monolayer transition metal dichalcogenides are ideal candidate materials for this purpose. Using density functional calculations, we illustrate that they exhibit not only exceedingly large magnetocrystalline anisotropy (MCA) but also colossal voltage modulation under external field. Especially, spins in some materials like $CrSe_2$ and $FeSe_2$, which is strongly preferred to in-plane orientation, can be totally switched to out-of-plane direction. The effect is attributed to the large band character alteration of transition metal *d*-states around the Fermi level by electric field. We further demonstrate that strain can also greatly change MCA, and can help to improve the modulation efficiency while combining with electric field.

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