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Prediction of two-dimensional van der Waals ferroelectric materials WENJUN DING, JIANBAO ZHU, University of Science and Technology of China, YANFEI GAO, University of Tennessee, DI XIAO, Carnegie Mellon University, YI GU, Washington State University, ZHENYU ZHANG, WENGUANG ZHU, University of Science and Technology of China — Based on density functional theory calculations, we discover a class of two-dimensional van der Waals ferroelectric materials with spontaneous out-of-plane electric polarization, and the orientation of the electric polarization can be reversed by a seemly lateral shift of a single atomic layer. We further find that the electronic structures of a bilayer of such two-dimensional ferroelectric materials can be switched to be either semiconducting or metallic, depending on their relative orientations of the electric polarization. This finding expand the family of the two-dimensional materials with ferroelectricity and offers new opportunities to tune the properties of van der Waals heterstructures for practical device applications.

Wenguang Zhu
University of Science and Technology of China

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