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Giant piezoelectricity of monolayer group IV monochalcogenides. RUIXIANG FEI, Department of Physics, Washington University, WENBIN LI, Research Laboratory of Electronics, Massachusetts Institute of Technology, JU LI, Department of Nuclear Science and Engineering and Department of Materials Science and Engineering, Massachusetts Institute of Technology, LI YANG, Department of Physics, Washington University — We predict enormous, anisotropic piezoelectric effects in intrinsic monolayer group IV monochalcogenides (MX, M=Sn or Ge, X=Se or S), including SnSe, SnS, GeSe, and GeS. Using first-principle simulations based on the modern theory of polarization, we find that their piezoelectric coefficients are about one to two orders of magnitude larger than those of other 2D materials, such as MoS2 and GaSe, and bulk quartz and AlN which are widely used in industry. This enhancement is a result of the unique "puckered" C2v symmetry and electronic structure of monolayer group IV monochalcogenides. Given the achieved experimental advances in the fabrication of monolayers, their flexible character, and ability to withstand enormous strain, these 2D structures with giant piezoelectric effects may be promising for a broad range of applications such as nano-sized sensors, piezotronics, and energy harvesting in portable electronic devices.

> Ruixiang Fei Washington Univ

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