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Ferroelectricity and Phase Transitions in two-dimensional materials RUIXIANG FEI, Department of Physics and Institute of Materials Science and Engineering, Washington University, St. Louis, Missouri 63130, USA, WEI KANG, HEDPS, Center for Applied Physics and Technology, and College of Engineering, Peking University, Beijing 100871, China, LI YANG, Department of Physics and Institute of Materials Science and Engineering, Washington University, St. Louis, Missouri 63130, USA — Ferroelectricity usually fades away as materials are thinned down below a critical value. We reveal that the unique ionic-potential anharmonicity can induce spontaneous in-plane electrical polarization and ferroelectricity in monolayer group-IV monochalcogenides MX (M= Ge, Sn; X= S, Se). An effective Hamiltonian has been successfully extracted from the parametrized energy space, making it possible to study the ferroelectric phase transitions in a single-atom layer. The ferroelectricity in these materials is found to be robust and the corresponding Curie temperatures are higher than room temperature, making them promising for realizing ultrathin ferroelectric devices of broad interest. We further provide the phase diagram and predict other potentially two-dimensional ferroelectric materials.

Ruixiang Fei
Washington University

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