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Peculiar Piezoelectricity in Two-Dimensional Materials CEM SEVIK, Department of Mechanical Engineering, Faculty of Engineering, Anadolu University, Eskisehir, TR 26555, Turkey, DENIZ CAKIR, Department of Physics and Astrophysics, University of North Dakota, Grand Forks, 58202, ND, USA, OGUZ GULSEREN, Department of Physics, Bilkent University, Bilkent, Ankara 06800, Turkey, FRANCOIS M. PEETERS, Department of Physics, University of Antwerp, Groenenborgerlaan 171, 2610 Antwerpen, Belgium — Recently, two dimensional materials with noncentrosymmetric structure have received significant interest due to their potential usage in piezoelectric applications. It has been reported by first principles calculations that relaxed-ion piezoelectric strain (d_{11}) and stress (e_{11}) coefficients of some transition metal dichalcogenide (TMDC) monolayers are comparable or even better than that of conventional bulk piezoelectric materials. Furthermore, e_{11} coefficient of MoS_2 has been measured as $2.9{\cdot}10^{-10}$ C/m, which agrees well with the theoretical calculations. In order to deeply investigate this potential, we have performed first-principles calculations and systematically investigated the piezoelectric properties of various single layer structures: TMDCs, transition metal oxides, and hexagonal group II-VI compounds. The results clearly show that not only the Mo- and W-based TMDCs but also the other materials with Cr, Ti, Zr and Sn exhibit highly promising piezoelectric properties. Moreover, d_{11}coefficient of some II-VI compounds have been predicted as quite larger than that of TMDCs and the bulk materials, α-quartz,w-GaN, and w-AlN which are widely used in applications.

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