Piezoelectricity in Magnetic 2D Materials

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Piezoelectric materials convert mechanical energy to electrical energy, and vice versa. A wide range of electromechanical devices relies on piezoelectric-based energy conversion. Being intrinsically nano-size, flexible two-dimensional (2D) piezoelectric materials can miniaturize these electromechanical devices e.g. nanoscale sensors, energy harvesters, and actuators. However, a large piezo-response is desired for any practical applications. Recently, based on Density Functional Theory (DFT) calculations, we have predicted that ferroelectric/multiferroelectric MOX_2 (M=Ti, V and X = F, Cl, Br) monolayers possess large in-plane stress (e_{11}) and strain (d_{11}) piezoelectric coefficients[1]. For example, $TiOBr_2$ monolayer has approximately one order of magnitude larger in-plane piezo-response ($e_{11} = 28.793\times10^{-10}$ C/m and d_{11} = 37.758 pm/V) than the widely studied piezoelectric 1H-MoS_2 monolayer. Furthermore, MOX_2 monolayers exhibit large d_{11} coefficient ranging from 29.028 pm/V to 37.758 pm/V, significantly higher than the d_{11} or d_{33} of traditional 3D piezoelectrics such as *w*-AlN (d_{33} = 5.1 pm/V) and *α*-quartz (d_{11} = 2.3 pm/V)[1]. MOX_2 monolayers possess a large d_{11} because of their low in-plane elastic constants and large e_{11}. Large Born effective charges (Z_{ij}) and atomic displacement in response to an applied strain ensure a large e_{11}. Note that multifunctional spintronic devices can utilize coupling between piezoelectricity and magnetism in 2D materials. However, piezoelectricity requires a non-centrosymmetric structure with an electronic band gap, whereas magnetism demands broken time-reversal symmetry. Most of the well-known 2D piezoelectric materials, e.g., 1H-MoS_2 monolayer, are not magnetic. Being intrinsically magnetic, semiconducting 1H-$LaBr_2$, 1H-VS_2 and VOX_2 monolayers can combine magnetism and piezoelectricity. We show the possibility of opening a new way of controlling piezoelectricity by changing the magnetic order such as changing antiferromagnetic to ferromagnetic, or vice versa. For example, a change in magnetic order can enhance (reduce) the piezo-response of 1H-$LaBr_2$ (1H-VS_2)[2].

References

[1] M. Noor-A-Alam and M. Nolan, ACS Appl. Electron. Mater., 4(2022), 850–855
[2] M. Noor-A-Alam and M. Nolan, Nanoscale, 14(2022), 11676-11683