

Origin and Enhancement of the Piezoelectricity in Monolayer Group IV Monochalcogenides Under Strain and in the Presence of Vacancies

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Abstract

Piezoelectric materials are a critical component in many electronic devices from the nanoscale to the macroscale. Monolayer group IV monochalcogenides can provide particularly large piezoelectric coefficients [1]. To investigate the origin of this strong piezoelectricity, we conduct an atomic-level analysis of the charge redistribution under mechanical strain. Our results show that it arises from charge transfer between strong and weak chemical bonds. We demonstrate that the piezoelectric coefficients can be substantially enhanced by mechanical strain and the presence of vacancies.

References

[1] R. Fei, W. Li, J. Li, and L. Yang, *Appl. Phys. Lett.*, 17 (2015) 173104

Figures

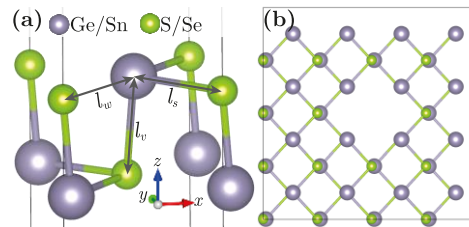


Figure 1: Crystal structure of the monolayer group IV monochalcogenides GeS, GeSe, SnS, and SnSe, where l_v , l_s , and l_w represent the bond lengths of the vertical, strong, and weak bonds, respectively. (b) Top view of a 4×4 supercell of SnSe with a pair of Sn and Se atoms removed (SnSe-v4).

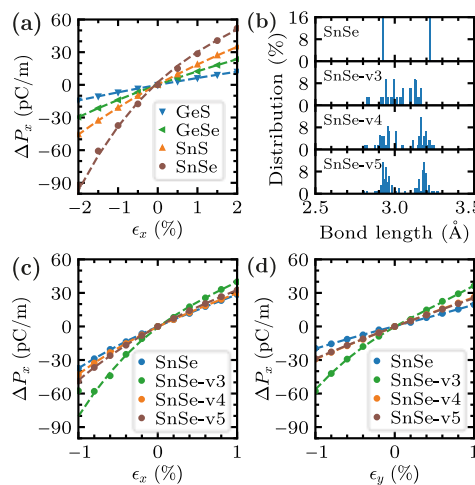


Figure 2: (a,c,d) Variation of the polarization under strain in pristine monolayer GeS, GeSe, SnS, and SnSe as well as in monolayer SnSe with Sn-Se vacancy. (b) Histograms of the intralayer bond lengths (l_s and l_w).