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Onset of out of plane ferroelectric polarization in ultra-thin Janus WSSe monolayer

Abstract

The search of ferroic ordering in a material attracted attention to the scienfitic commuinity and recently combining more than one ferroic ordering in a single system has shown potential for new functional devices. Recently, Shirodkar et al. [1] showed the out of plane ferroelectric polarization ~0.28 μC/cm^2 in the 1T phase of MoS_2 monolayer using the density functional theory. Bruyer et al. [2] also predicted the ferroelectric polarization in the 1T phase of the MX_2 (M = Mo, W; X = S, Se Te) in the range of 0.10 μC/cm^2 to 0.23 μC/cm^2. In contrast to 1T phase, WS_2 and WSe_2 monolayers in 1H phase do not exhibit ferroelectric polarization because of centrosymmetric nature of the monolayer. Janus WSSe monolayer breaks the out of plane symmetry intrisically in C_{3v} point group together with 1H crystal structure.In this work, we are reporting for the first time onset of out plane ferroelectric ordering in Janus WSSe monolayer, Fig 1, using density functional theory with ~ 0.33 μC/cm^2 ferroelectric polarization. The ferroelectric polarization is attributed to replacement of one site of chalcogen (say S) with another chalcogen atom (say Se) of different atomic radii. This breaks down the inversión symmetry intrisically in WSSe Janus layer. We further investigated the impact of external biaxial tensile and compressive strains and observed that tensile strain leads to a reduction, whereas compressive strain shows enhancement in the ferroelectric polarization.The present work will also discuss about the microscopic origin of the onset of polarization and its correlation with charge densities and other electronic properties.

References

[1] Shirodkar, Sharmila N., and Umesh V. Waghmare. "Emergence of ferroelectricity at a metal-semiconductor transition in a 1 T monolayer of MoS 2." *Physical review letters* 112.15 (2014): 157601.

[2] Bruyer, Emilie, et al. "Possibility of combining ferroelectricity and Rashba-like spin splitting in monolayers of the 1 T-type transition-metal dichalcogenides M X 2 (M= Mo, W; X= S, Se, Te)." *Physical Review B* 94.19 (2016): 195402.

Figure:

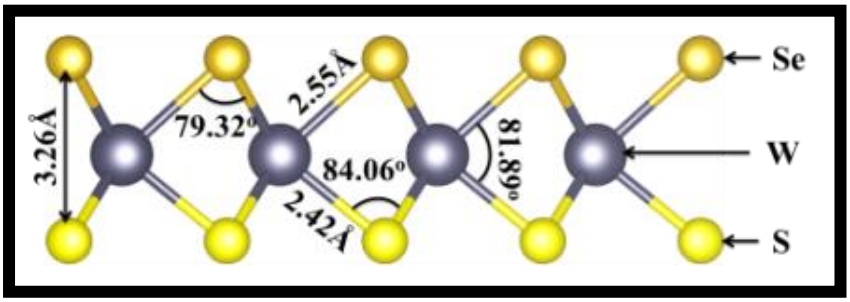

Figure.1 Schematic view and optimized structural parameters of Janus WSSe monolayer