

Physical properties of ferroelectric group-IV monochalcogenide monolayers

Salvador Barraza-Lopez

University of Arkansas and MonArk Quantum Foundry, Fayetteville, Arkansas, United States
sbarraza@uark.edu

Group-IV monochalcogenide monolayers are a novel, experimentally available group of two-dimensional materials that lack centro-symmetry, making them ultrathin ferroelectrics with an in-plane intrinsic electric polarization [1]. In this talk, I will first introduce the three experimentally available members of this family, demonstrating their ferroelectric behaviour [2]. Afterwards, I will describe theoretical efforts carried out within my group to understand their thermally-driven two-dimensional structural phase transitions [3-6]. I will then cover additional phenomena, such as thermoelectric properties across said phase transition [7], and the elastic properties of these materials at finite temperature [8]. Highlights of a five-year collaborative effort with teams in China and Germany within the context of these materials will be provided along the way. This work is being funded by the US Department of Energy (Early Career Award DE-SC001613; and DE-SC0022120; calculations carried out at NERSC, a DOE User Facility under Contract No. DE-AC02-05CH11231).

References

- [1] Discovery of robust in-plane ferroelectricity in atomic-thick SnTe. K Chang et al. *Science* **353**, 274 (2016).
 - [2] Colloquium: Physical properties of group-IV monochalcogenide monolayers. S Barraza-Lopez, BM Fregoso, JW Villanova, SSP Parkin, K Chang. *Rev. Mod. Phys.* **93**, 011001 (2021).
 - [3] Structural phase transition and material properties of few-layer monochalcogenides. M Mehboudi, et al. *Phys. Rev. Lett.* **117**, 246802 (2016).
 - [4] Two-dimensional disorder in black phosphorus and monochalcogenide monolayers. M Mehboudi, et al. *Nano Lett.* **16**, 1704 (2016).
 - [5] Tuning the ferroelectric-to-paraelectric transition temperature and dipole orientation of group-IV monochalcogenide monolayers. S Barraza-Lopez, TP Kaloni, SP Poudel, P Kumar. *Phys. Rev. B* **97**, 024110 (2018).
 - [6] Theory of finite-temperature two-dimensional structural transformations in group-IV monochalcogenide monolayers. JW Villanova, P Kumar, S Barraza-Lopez. *Phys. Rev. B* **101**, 184101 (2020).
 - [7] Anomalous thermoelectricity at the two-dimensional structural transition of SnSe monolayers. JW Villanova, S Barraza-Lopez. *Phys. Rev. B* **103**, 035421 (2021).
 - [8] Elasticity of 2D ferroelectrics across their paraelectric phase transition. JW Villanova, S Barraza-Lopez. Under review (2021).
-

Figures



Figure 1: Structural snapshot of a prototypical group-IV monochalcogenide monolayer at finite temperature.
