Monolayer of 1TMoS_2: The Thinnest Ferroelectric?

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Ferroelectric crystals exhibit an electric dipole moment (spontaneous polarization) even in the absence of an external electric field. When heated, ferroelectric materials transform at the ferroelectric transition temperature to the centrosymmetric and non-polar paraelectric phase. The macroscopic electric polarization in ferroelectrics can be switched by the application of external electric fields. Hence, their films are used in various devices such as sensors, actuators and memories. As ferroelectric ordering of dipoles oriented perpendicular to the surface of an ultrathin film is suppressed by their depolarization field, ferroelectricity has been shown to disappear below film thicknesses of 24 Å in $BaTiO_3$, 8 Å in $PbTiO_3$ and 10 Å in polymer films. However, truly 2-dimensional materials such as graphene, hexagonal boron nitride and MoS_2 have not been explored for its existence. Here, we predict the emergence of unexpected, yet robust ferroelectricity (with polarization perpendicular to the plane) in the 1T polytype of MoS_2 as it undergoes a transition from metallic to insulating state by using a combination of first-principles and Landau theoretical analysis. We show that it originates from the geometry of electronic Fermi surface through a strong coupling of d-orbitals of Mo with valley phonons that induce an effective electric field. Our prediction of a 2-dimensional ferroelectric semiconductor opens up a new class of nanoscale dipotronic devices based on MoS_2, and we propose XNOR, NAND and OR logic gates within a single transistor structure [1].

References

[1] Sharmila N. Shirodkar and Umesh V. Waghmare, PRL **112**, 157601 (2014).