1T-distorted Phase Janus MoSTe: A Piezoelectric Single-Layer

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Recently synthesized single-layer Janus MoSSe[1] has been also predicted to possess out-of-plane piezoelectric property[2]. We predict the dynamical stability of a 1T-distorted phase of Janus MoSTe (see Fig. 1(b)) structure and investigate its electronic, elastic, vibrational, and piezoelectric properties and compare them with those for the 1H phase. 1T-distorted MoSTe is found to be a semimetal while the 1H phase is an indirect band gap semiconductor with a band gap of 1.37 eV which is incontrast to the 1H phases of MoS_2 and $MoTe_2$. In addition, 1T-distorted phase is shown to exhibit a small anisotropy in terms of the in-plane stiffness due to the presence of the Mo-Mo chains. Moreover, its Raman spectrum possesses 15 Raman active modes from which it is possible to distinguish the two phases. We further analyze the relaxed-ion piezoelectric tensors and found that the non-piezoelectric 1T-distorted MoS_2 and $MoTe_2$ become piezoelectric in 1T-distorted Janus MoSTe due to created out-of-plane anisotropy. We propose that it would be feasible to synthesize the 1T-distorted phase of MoSTe by replacing Te atoms by S atoms in 1T-distorted $MoTe_2$.

Figures

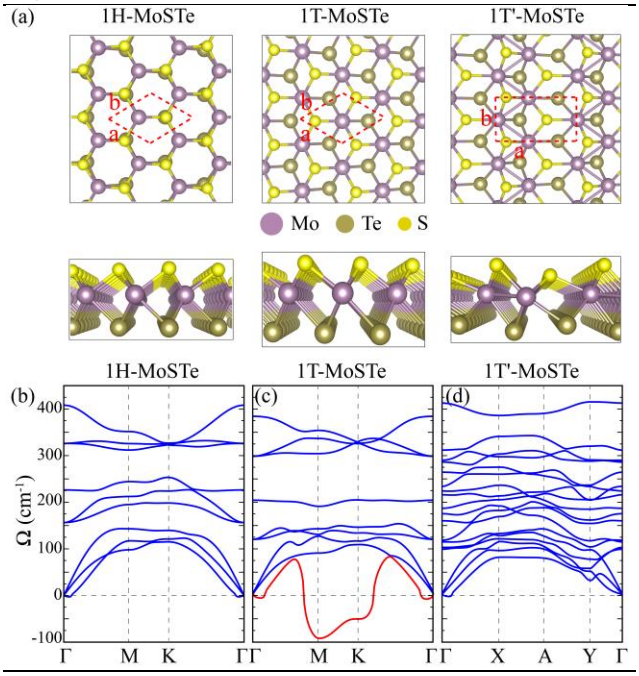

Figure 1: Three Janus MoSTe structures; (a) Top and side view of different phases. (b) The corresponding phonon-band dispersions. The red-curve phonon branch shows the dynamical instability of the 1T phase.

References

[1] A.-Y. Lu *et al.*, Nat. Nanotech., **12** (2017) 744.

[2] L. Dong *et al.*, ACS Nano, **11** (2017) 8242.