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***Ab initio* study on ferroelectric instability induced by relativistic effects in PbTe**[1] JINWOONG KIM, SEUNG-HOON JHI, POSTECH — A recent study [E. S. Bozin *et al.*, Science 330, 1660 (2010)] reported unusual ferroelectric instability in lead chalcogenides at heating, which is contrast to typical ferroelectric transitions that occur at cooling. This study explains the emergence of local dipole formation due to the softening of transverse optical (TO) phonon modes. However, standard first-principles calculations do not support the phonon softening (imaginary frequency). Here, we present that the spin-orbit interaction should be included in the calculations to correctly produce the instability and that, as such, thermal expansion leads to the softening in TO phonon modes. Another controversial finding in experiment that the frequency of TO mode is finite and increases with temperatures can be explained if anharmonic effects are considered together with the spin-orbit interaction. Our study shows that the spin-orbit interaction can be critical for the structural stability and thus affect the thermoelectric or structural phase transition.

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