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Topological phase transition induced by atomic displacements in PbS and PbTe JINWOONG KIM, Dept. of Physics, POSTECH, SEUNG-HOON JHI, Dept. of Physics and Division of Advanced Materials Science, POSTECH — Discovery of 3D topological insulator initiates exploration of finding new materials having topological insulating phase or mechanisms for topological phase transitions. Introducing interactions or strains into non-interacting electron systems, for example, can produce non-trivial topological phases in them otherwise having trivial band insulating phase at equilibrium conditions. Using first-principles methods, we study emerging topological phases in band insulating PbS and PbTe, which are induced by selective atomic displacements. Phonon modes corresponding to the displacements are identified and conditions of inducing the topological phase transition are suggested. We show that surface states develop flickering Dirac cones at band-inversion k-points upon dynamic atomic displacements with sufficient amplitude. Our results demonstrate that elementary excitation modes like phonon can induce topological phases in trivial band insulators.

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