Ab-initio Simulations of Coherent Phonon-Induced Pumping of Carriers in Zirconium Pentatelluride

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Laser-driven coherent phonons can act as modulated strain fields and modify the adiabatic ground state topology of quantum materials. Here we use time-dependent first-principles and effective model calculations to simulate the effect of the coherent phonon induced by strong terahertz electric field on electronic carriers in the topological insulator $ZrTe_5$. We show that a coherent A_{1g} Raman mode modulation can effectively pump carriers across the band gap, even though the phonon energy is about an order of magnitude smaller than the equilibrium band gap. We reveal the microscopic mechanism of this effect which occurs via Landau-Zener-Stückelberg tunneling of Bloch electrons in a narrow region in the Brillouin zone center, where the transient energy gap closes when the system switches from strong to weak topological insulator. The quantum dynamics simulation results are in excellent agreement with recent pump-probe experiments in $ZrTe_5$ at low temperature.

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