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**The intrinsic coupling of polarization with terahertz pulses in a ferroelectric nanowire**[1] KIMBERLY SCHULTZ, Carthage College, RYAN HERCHIG, KEVIN MCCASH, INNA PONOMAREVA, University of South Florida — We use first-principles-based molecular dynamics simulations to study the interaction of a terahertz (THz) radiation with polarization in a ferroelectric ultrathin nanowire made of a lead zirconate titanate alloy. In our computational experiment, a 12 nm thick nanowire is first annealed down to temperature of 300 K and then subjected to a wide variety of THz pulses which differ in width, strength and frequency. Such nanowire develops an electrical polarization along the nanowire axial direction which couples strongly with incoming THz radiation. The atomistic resolution of our computational experiments allows us to trace the intrinsic polarization response and energy propagation/dissipation mechanisms that occur at the scale of femtoseconds. Our simulations were carried out under MVE and MVT conditions and the results did not vary significantly between the two ensembles. We further explore how the unique features of such response could be utilized in an ultrafast THz nanoswitches.

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