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**Phonon mediated ultrafast spin relaxation of a valley-polarized electron in monolayer MoS2** DONGBIN SHIN, HOSUB JIN, NOEJUNG PARK, Ulsan National Institute of Science and Technology — The excited state of a particularly selected spin- and valley-polarized electron is gathering growing interest in terms of the coupling between different degrees of freedom and also in the perspective novel device functionality. The measurement of monolayer of MoS2 is quite much matured, and the time scales of spin relaxation, inter-valley scattering, intra-valley scattering, and electron-hole recombination have been analyzed through circularly polarized pump-prove experiments. The spin relaxation is believed to occur within 100 fs which is distinctly faster than all the other degrees of freedom. Here, we use the real-time propagation time-dependent density functional theory (rtp-TDDFT) method to investigate the microscopic origin of the spin dynamics. We present that the specific phonon, that breaks the mirror symmetry of 2H-phase of MoS2, sharply causes the precession of spins through the strong spin-orbit interaction. Thus the incoherent population of such phonons can cause the temperature-dependent relaxation of the spin polarization. We also discuss the general effect of oscillating magnetic field carried by phonons in the strong spin-orbit coupled solid system.

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