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Role of the electron phonon coupling in pump-probe experiments on 1T-TaS_2 JENNI PORTMAN, BIN HWANG, DAT THANH DO, FARAN ZHOU, TZONG-RU TERRY HAN, CHONG-YU RUAN, S.D. MAHANTI, PHILLIP DUXBURY, Michigan State University — 1T-TaS_2 is a transition-metal layered compound that shows unique electronic properties and phase transitions, including charge density wave (CDW) formation. By performing pump-probe experiments, the CDW state can be suppressed and its recovery can be investigated as a function of time delay and laser parameters. We perform density functional theory calculations of the band structure of 1T-TaS_2 to explain the microscopic quantum mechanical origin of this behaviour. By calculating the phonon band structure and the phonon-electron coupling, we quantify the contribution of lattice relaxation at various laser frequencies. We also perform calculations of the absorption spectrum using time-dependent DFT and show how an interplay of the phonon and electron degrees of freedom can explain the different timescales and structural properties involved in the response of CDW materials to laser excitations.

Jenni Portman
Michigan State University

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