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Pressure-Dependent Optical and Vibrational Properties of Monolayer Molybdenum Disulfide AVINASH NAYAK, UT Austin, TRIBHUWAN PANDEY, Materials Research Center, Indian Institute of Science, Bangalore, 560-012, India, DAMIEN VOIRY, Department of Materials Science and Engineering, Rutgers University, JIN LIU, Department of Geological Sciences, The University Of Texas at Austin, SAMUEL MORAN, ANKIT SHARMA, CHENG TAN, UT Austin, CHANG-HSIAO CHEN, Institute of Atomic and Molecular Sciences, Academia Sinica, Taipei, 10617, Taiwan, LAIN-JONG LI, Physical Science and Engineering Division, King Abdullah University of Science & Technology (KAUST), Thuwal 23955, Saudi Arabia, MANISH CHHOWALLA, Department of Materials Science and Engineering, Rutgers University, JUNG-FU LIN, Department of Geological Sciences, The University Of Texas at Austin, ABHISHEK SINGH, Materials Research Center, Indian Institute of Science, Bangalore, 560-012, India, DEJI AKINWANDE, UT Austin, DEJI AKINWANDE TEAM, ABHISHEK SINGH TEAM, LANCE LI COLLABORATION, MANISH CHHOWALLA COLLABORATION, HPSTAR COLLABORATION — Controlling the band gap by tuning the lattice structure through pressure engineering is a relatively new route for tailoring the optoelectronic properties of two dimensional (2D) materials. Here we investigate the electronic and lattice vibrational dynamics of the distorted monolayer 1T-MoS_2 (1T') and the monolayer 2H-MoS_2 *via* a diamond anvil cell (DAC) and density functional theory (DFT) calculations. The direct optical band gap of the monolayer 2H-MoS_2 increases by 11.7% from 1.85 eV to 2.08 eV, which is the highest reported for a 2D transition metal dichalcogenide (TMD) material.

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