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Piezoelectricity Enhancement and Band Structure Modification of Single Atomic Shift in MoS_2 Supercell Monolayer[1] FELIX JAETAE SEO, SHENG YU, QUINTON RICE, SHOPAN HAFIZ, BAGHER TABIBI, Hampton University, QILIANG LI, George Mason University, HAMPTON UNIVERSITY TEAM, GEORGE MASON UNIVERSITY COLLABORATION — A monolayer of transition metal dichalcolgenides (TMDCs, TM: Mo, W, DC: S, Se, Te) has second-order nonlinearity including piezoelectricity responding to an external field due to spatial inversion asymmetry. The intrinsic piezoelectric coefficient (e_{11}) of MoS_2 without any atomic shift has ˜298 pC/m, where e_{11} indicates the sum of ionic and electronic polarizations along the armchair direction responding to the uniaxial atomic shift along the armchair direction. The piezoelectric coefficients (e_{11}) of MoS_2 supercell with a single atomic shift of Mo- and S-ion positively (20%) along the armchair direction were increased to ˜350 pC/m and ˜305 pC/m, respectively. Meanwhile, the piezoelectric coefficients (e_{11}) of MoS_2 supercell with a single atomic shift of Mo- and S-ion positively (20%) along the zigzag direction have ˜330 pC/m. The bandgap energy at the K point in the first Brillion zone of a single atomic shift either Mo- and S-ions positively (20%) along the armchair direction in the MoS_2 atomic cell is largely reduced to ˜0.06 eV compared to the intrinsic bandgap (1.96 eV) of MoS_2 without atomic stain. The large piezoelectricity enhancement and bandgap modification due to a single atomic shift in TMDCs may open astonishing scientific research and applications including quantum information processing and optomechanics in the pico-scale atomic layer.

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