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Mechanical Modulation of Tunneling Current in Transition Metal Dichalcogenides Heterostructures: A First Principles Study MARCELO KURODA, Auburn University — Recent experiments in MoS_2 heterostructures reported that out-of-plane tunneling piezoresistivity (TPR) – mechanical modulation of the tunneling current – achieves sensitivities of one decade per Å displacement. Owing to their nanometer scale, a quantitative theoretical framework providing the TPR structure-property relationship is necessary to further improve sensitivities. To this end, first principles calculations within density functional theory are used to characterize the phenomenon in MoX_2 (with X = S, Se). The TPR is quantified in relation to electrode composition and film thickness showing remarkable agreement with experiments. The origin of the TPR is attributed to the heterostructure compliance rather than band alignment changes with strain, and differs from mechanisms in other nanometer-thick bulk films. Large work function metals (Pt, Au) are singled out as best candidates for enhanced TPR gauges due to weak bonding and negligible thermionic emission; compliant bilayers show larger stress-sensitivity than monolayers. By accounting for the atomistic details and material composition of 2D material-based heterostructures, this work has the potential to advance sensor and nano-electro-mechanical system technologies.

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