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Electro-vibronic Coupling Effects on "Intrinsic Friction" in Transition Metal Dichalcogenides[1] ANTONIO CAMMARATA, Czech Technical University in Prague, TOMAS POLCAR, Czech Technical University in Prague and University of Southampton — One of the main difficulties in understanding and predicting frictional response is the intrinsic complexity of highly non-equilibrium processes in any tribological contact, which include breaking and formation of multiple interatomic bonds between surfaces in relative motion. To understand the physical nature of the microscopic mechanism of friction and design new tribologic materials, we conducted a systematic quantum mechanic investigation at the atomic scale on prototipical Van der Waals MX_2 (M=Mo, W; X=S, Se, Te) Transition Metal Dichalcogenides under variable load. We combined the structural and dynamic information from group theoretical analysis and phonon band structure calculations with the characterisation of the electronic features using non-standard methods like orbital polarization and the recently formulated bond covalency and cophonicity analyses. We formulated guidelines on how to engineer macroscopic friction at nanoscale, and finally applied them to design a new Ti-doped MoS_2 phase. The formulated protocol can be promptly used for the design of new materials with diverse applications beyond tribology.

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