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**Kinetics and atomic mechanisms of rapid semiconductor-to-metal transitions in monolayer TMDCs**[1] ARAVIND KRISHNAMOORTHY, CACS, USC, LINDSAY BASSMAN, CACS, Dept. of Physics Astronomy, USC, AIICHIRO NAKANO, RAJIV KALIA, PRIYA VASHISHTA, CACS, Depts. of Physics Astronomy, Computer Science, and Chemical Engg. Material Science, USC, HIROYUKI KUMAZOE, MASAAKI MISAWA, FUYUKI SHIMOJO, Dept. of Physics, Kumamoto University — Rapid and controllable transitions between semiconducting (H) and metallic (T') phases of monolayer transition-metal dichalcogenides are of interest for 2D electronics. However, theoretical studies have been limited to calculations of thermodynamic stability of H and T' phases, while experimental investigations have uncovered only slow thermally-activated transitions that occur over $10^3 - 10^4$ seconds. Here, we demonstrate, through a combination of DFT and non-adiabatic QMD, softening of phonon modes located at the Brillouin zone boundary, thus exposing a hitherto unknown low barrier pathway for the H-T' phase transformation. We compare the fast kinetics of this new mechanism to previous strategies for improving the H-T' phase transition by quantifying phase transition activation barriers in strained, charge- and donor-doped monolayers using NEB. We discuss implications of this pathway in enabling fast phase transitions through irradiation for use in 2D electronics and non-volatile memories.

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