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Structural and electronic phase transitions of $MoTe_2$ induced by Li ionic gating

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Phase transition induced by field effect is a superior property of low dimensional systems. Huge doping concentration accessible via ionic gating enables to observe structural and electronic changes in those systems beyond the quasiparticle energy renormalization. Monolayer $MoTe_2$ has semiconducting and semimetallic phases with small energy difference, and the relative stability is readily reversed by gating. By first-principles calculations, we investigate the changes in atomic structure, electronic structure, and relative stability of two phases induced by Li ionic gating. To model Li ionic gating, we employ two approaches; one is direct adsorption of Li on $MoTe_2$ and the other is introducing non-contacting Li plate over $MoTe_2$. We show phonon instability in H-phase of $MoTe_2$ with increasing the amount of charge transfer from Li, which implies a large electron-phonon coupling in the system resulting in a charge density wave state. Structural distortion is also observed in highly doped T_d phase. The transition energy barrier from distorted H phase to distorted T_d phase is reduced considerably compared to that of pristine $MoTe_2$.