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Electron/Hole-phonon scattering and intrinsic carrier mobility in 2D transition metal dichalcogenides(TMDs)[1] ZHENGHE JIN, XIAODONG LI, BYOUNG-DON KONG, JEFFREY MULLEN, KI WOOK KIM, North Carolina State Univ — We have investigated electron/hole-phonon scattering mechanism in 2D transition metal dichalcogenides using a first-principles approach. Specifically, 2D TMDs, i.e., monolayer MX_2 (M=Mo and W; X=S and Se) material are investigated. The scattering rates are calculated using Density Functional Theory (DFT) and Density Functional Perturbation Theory (DFPT) and intrinsic electron/hole-mobility is obtained though full band Monte Carlo carrier transport simulation. Then, the parameters for the deformation potential model are extracted from the first principle's transport studies for practical purposes. Our calculation reveals WS_2 has the largest mobility among the investigated TMDs. At room temperature, the electron mobility of WS_2 is 300 cm^2/Vs, which is smaller than that of usual bulk semiconductor. Contrary to this, the hole mobility of WS_2 turns out to be over than 800 cm^2/Vs, which is even higher than that of bulk silicon, which provides a good opportunity of high-performance pMOSFET. Our work examines the electronic transportation property of 2D TMD material from first-principles approach and demonstrates the importance of electron/hole-phonon scattering in those materials and provides optimal channel material for future field effect transistor.

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