Electron-phonon coupling dynamics for tunable bandgap of transition metal dichalcogenide atomic layers

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The atomic layers of 2-dimensional transition metal dichalcogenides (TMDCs, MX_2; M=Mo or W; X=S, Se, or Te) are of great interest in the areas of optoelectronic and photonic applications due to the bandgap conversion from direct for monolayer and indirect for bilayer or multilayer; unique properties of valley orbital, spin, and optical helicity; and compositional tuning of exciton bandgaps in visible and near-infrared region. In this work, the average acoustic phonon energy involved in the electron-phonon interaction as well the coupling strength between electrons and phonons is analyzed using the O'Donnell and Chen relation for the temperature-dependent bandgap of TMDCs. The analysis shows that as the temperature is increased the exciton band energy is decreased. When the electron-phonon coupling strength is large (small) the tunability of exciton bandgap is wide (narrow) for a constant acoustic phonon energy. Weak electron-phonon coupling (S=2) leads to a linear decrease in the bandgap energy for temperature above ~85 K but strong coupling (S=30) above ~60 K. The bandgap was changed from 2 eV to 0.5 eV for both weakly and strongly coupled electrons, however, for a constant electron-phonon coupling strength, large (small) acoustic phonon energy results in narrow (wide) tunability of the bandgap. The ability to control the exciton bandgap through the electron-phonon interaction and average acoustic phonon energy at various temperatures leads to tunable optoelectronic and photonic devices based on 2-dimensional TMDCs. Acknowledgement: This work at HU is supported by ARO W911NF-15-1-0535, NSF HRD-1137747, and NASA NNX15AQ03A.

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