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Electron-Phonon Coupling and Photoluminescence in monolayer MoS_2[1] NEHA NAYYAR, VOLODYMYR TURKOWSKI, DUY LE, TALAT RAHMAN, University of Central Florida — We have carried out first principles calculations of the photoluminescent properties of monolayer MoS_2 using density functional theory. In particular, we have analyzed the role of electron-phonon interactions in the photoluminescence process. Phonon dispersion curves calculated using density functional perturbation theory served as the basis for the evaluation of the system electron-phonon coupling, which in turn was used to calculate electron self-energy and the electron spectral function within the Eliashberg approach. We find that the resulting photoemission spectrum is in good agreement with experimental data. We pay special attention to the ultrafast relaxation of the electron system as manifested by the electron-phonon coupling and evaluate the ultrafast photoluminescence of the excited system by using the two-temperature model. It is shown that similar to graphene, MoS_2 may demonstrate significant ultrafast photoluminescence.

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