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Ab-initio study of the temperature effects on the optical properties of transition metal dichalcogenides ALEJANDRO MOLINA-SANCHEZ, Physics and Material Sciences Research Unit, University of Luxembourg, MAURIZIA PALUMMO, Dipartimento di Fisica, University of Rome Tor Vergata, Italy, ANDREA MARINI, Istituto di Struttura della Materia, Consiglio Nazionale delle Ricerche, Monterotondo, Italy, LUDGER WIRTZ, Physics and Material Sciences Research Unit, University of Luxembourg — Research on ultra-thin two-dimensional materials has been booming since the discovery of graphene along with its interesting physical properties. The transition metal dichalcogenides as MoSare gaining considerable attention due to their potential application in photovoltaics and nanoscale transistors. The optical properties of these layered materials depend strongly on the number of layers. The paradigmatic example is the transition from indirect to direct bandgap when we change from multi-layer to single-layer MoS. In this work, we study the effects of the electron-phonon interaction on the optical properties of single-layer MoS. In the framework of the GW method we calculate the contribution of the electron-phonon coupling to the self-energy. This allows us to calculate the zero-point re-normalization of the quasi-particle energies and to include temperature effects. We discuss the bandgap dependence on the temperature, and the change in the linewidth of the quasi-particle states. The impact of temperature on the exciton states is also addressed.

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