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Theoretical study of luminescence spectrum of exciton in monolayer transition metal dichalcogenides; The role of intervalley Coulomb interaction and dynamical screening. DINH VAN TUAN, Department of Electrical and Computer Engineering, University of Rochester, HANAN DERY, Department of Electrical and Computer Engineering Department of Physics and Astronomy, University of Rochester — We investigate the luminescence properties of excitons in monolayer transition metal dichalcogenides in order to elucidatethe experimental results and the differences in the spectrum of MoSe2 and WSe2. We find that the experimental results can be explained only when incorporating dynamical screening and intervalley Coulomb interaction in the Bethe-Salpeter Equation (BSE) of the electron-hole pair Green's function. In the first step of our numerical scheme, the pair Green's function is evaluated at Matsubara frequencies, followed in the second step, by analytical continuation to the real axis using a Pade approximation. The obtained results agree far better with the experimental data compared with the solution of the BSE when using a statically screened potential.

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