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Ab initio studies of excitations in monolayer black phosphorus[1]
TOBIAS FRANK, MARCIN KURPAS, MARTIN GMITRA, University of Regensburg, RENE DERIAN, IVAN STICH, Inst. of Physics, Slovak Academy of Sciences, JAROSLAV FABIAN, University of Regensburg — Monolayer black phosphorus, or phosphorene, represents an ideal system to study many-body electron-electron and electron-hole interactions due to its strong anisotropy driven 1d electronic nature. In particular, the size of the fundamental band gap value and excitonic binding energies remain unresolved given the different gap values of 1.6 to 2.4 eV [1] obtained by many-body GW calculations. We present our contribution to this issue studying excitations in phosphorene employing quantum monte carlo (QMC) calculations. We show the evolution of finite size effects of the fundamental and optical gap, with respect to relatively large supercell sizes in the theoretical framework of diffusion monte carlo (DMC) explicitly including electronic correlations. Our studies point to a significant influence of electron correlation on the fundamental gap as well as to a strong anisotropic nature of the excitonic state. Furthermore we address the question of a multiconfigurational ground state in monolayer black phosphorus. [1] A. N. Rudenko, Shengjun Yuan, and M. I. Katsnelson, Phys. Rev. B 92 085419 (2015)

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