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Tuning the exciton energy in single and multi-layer black phosphorus by strain and electric field FRANCOIS PEETERS, DENIZ CAKIR, Universiteit Antwerpen, Dept. Physics, B-2020 Antwerpen, ANDRE CHAVES, UFC, Fortaleza, Brazil, HASAN SAHIN, Universiteit Antwerpen, Dept. Physics, B-2020 Antwerpen, CMT COLLABORATION — The effect of strain on the electronic and optical properties of single layer black phosphorus is investigated using first principles calculations. Biaxial strain is able to tune the optical band gap from 0.38 eV (at -8% strain) to 2.07 eV (at 5.5%). The exciton binding energy is found to be 0.40 eV for compressive biaxial strain of -8% and becomes 0.83 eV for tensile strain of 4%. The stack effect in the exciton energy is obtained by direct diagonalization of the effective mass Hamiltonian. The dependence on the number of phosphorus layers and the strength of the electric field is investigated. Band anisotropy becomes evident in the direction dependent field induced polarizability of the exciton.

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