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First Principles Absorption Spectra of Group IB and IIB Atoms and Dimers KOPINJOL BAISHYA, SERDAR OGUT, University of Illinois at Chicago — We present absorption spectra of group IB and IIB atoms and dimers, obtained with two state-of-the-art computational methods using ab initio pseudopotentials: the many body perturbation technique GWBSE and the time-dependent density functional theory with the local density approximation (TDLDA). We compare the GWBSE and TDLDA spectra with each other and with available experimental data. A recent study has shown that semi-core s and p states are essential to reproduce accurate quasiparticle energies within the GW theory.[1] We extend this investigation to the case of optical excitations and examine the effect of semi-core states on the absorption spectra by carrying out TDLDA and GWBSE computations with standard and semi-core pseudopotentials. [1] M.Tiago, J.C.Idrobo, S.Ogut, J.Jellinek, and J.R.Chelikwosky, Phys. Rev. B 79, 155419 (2009).

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