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Optical properties of alkali halide crystals from all-electron hybrid-exchange TD-DFT calculations ROSS WEBSTER, Imperial College, LEONARDO BERNASCONI, STFC Rutherford Appleton Laboratory, NICHOLAS HARRISON, Imperial College — I will present a study of the electronic and optical properties of a series of alkali halide crystals, based on a recent implementation of(hybrid) TD-DFT in the all-electron Gaussian basis set code CRYSTAL [1]. This TD-DFT implementation includes on-site correlation and long range electron-hole interactions by including non-local Fock exchange in the functional. I will examine in particular, the impact of the Gaussian basis set size and quality on the prediction of the band gap, optical gap, and exciton binding energy of these systems, expanding on our previous work [2]. I will show that the polarisability criterion proposed by Rappoport and Furche for molecular systems [3], can be used to converge calculated excited-state properties with the basis set size for periodic systems. I will compare results from CRYSTAL calculations with GW+BSE calculations, previous plane-wave pseudopotential estimates and with experimental data. Finally, I will explore the potential for development of this method, including choice of exchange-correlation kernel, and our current work on a wide range of systems.

[1]: www.crystal.unito.it
[2]: L. Bernasconi et al., J. Phys.: Conf. Ser., 367, 012001 (2012)
[3]: D. Rappoport and F. Furche, J. Chem. Phys, 133, 134105 (2010)

Ross Webster
Imperial College

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