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Time-dependent density-functional approach for exciton binding energies ARITZ LEONARDO[1], Department of Applied Physics II, UPV-EHU, Leioa, Spain, AITOR BERGARA[2], Deparment of Condensed Matter Theory, UPV-EHU, Leioa, Spain — Optical processes in insulators and semiconductors, including excitonic effects, can be described in principle exactly using time-dependent density-functional theory (TDDFT). Ullrich and co-workers adapted the Casida equation formalism for molecular excitations to periodic solids, which allows to obtain in a direct way, exciton binding energies without having to evaluate the response function. However, in this type of calculations the problem always arises from the lack of proper long-range behavior of the exchange correlation kernels in general. From a computational point of view, the kernels that exhibit Coulomb like tails need a special attention in periodic solids. More recently, Sundararaman and Arias developed an original and efficient method based on the Minimum Image Convention (MIC) in which Coulomb type interactions are truncated on Wigner-Seitz super-cells for the calculation of exchange energies of periodic solids. We have implemented this numerical scheme for the direct calculation of exciton binding energies of various small- and large-gap semiconductors, as the earlier mentioned Casida formalism resembles Fock type exchange integrals.

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