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Optical conductivity of GaP alloys studied by hybrid-density functional theory YOSHIHIRO GOHDA, SHINJI TSUNEYUKI, The University of Tokyo — Highly-mismatched semiconductor alloys are promising to produce multiple gaps utilizing wider frequency range of the solar spectrum. Quantitative first-principles calculations of the optical conductivity, which is of importance to access the performance of solar cells, are out of reach for the standard generalized gradient approximation (GGA) in density functional theory (DFT) due to well-known underestimation of the band gap. To overcome this problem, hybrid-DFT scheme is quite useful, which incorporates nonlocality of the exchange interaction reducing the self-interaction error in the GGA. In this work, highly-mismatched GaP alloys are studied as candidates for intermediate-band solar cells, where the optical conductivity is calculated on the basis of hybrid-DFT combined with time-dependent perturbation theory. Thanks to the practical computational costs of hybrid-DFT compared with the GW approximation, structures with realistic dopant concentrations are handled with 216-site supercells. Ideal composition of alloys in the sense of active optical transition energies and the formation energy are compared, where calculated results propose that the optimal doping condition is Mg-O co-doping [Y. Gohda and S. Tsuneyuki, Appl. Phys. Lett., in press.]

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