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Accurate effective masses from first principles JONATHAN LAFLAMME JANSSEN, XAVIER GONZE, Université catholique de Louvain, Institute of Condensed Matter and Nanosciences, Nanoscopic Physics — The accurate ab initio description of effective masses is of key interest in the design of materials with high mobility. However, up to now, they have been calculated using finite-difference estimation of density functional theory (DFT) electronic band curvatures. To eliminate the numerical noise inherent to finite-difference and obtain an approach that is more suitable for material design using high throughput computing, we develop a method allowing to obtain the curvature of DFT bands using Density-Functional Perturbation Theory (DFPT), taking a change of wavevector as a perturbation. Also, the inclusion of G_0W_0 corrections to DFT bands in our method will be presented.

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