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**Lattice polarization contribution in the quasi-particle self-consistent GW approach.**[1] WALTER R. L. LAMBRECHT, CHURNA BHANDARI, Case Western Reserve University, MARK VAN SCHILFGAARDE, King's College — The lattice polarization contribution to the screening of the screened Coulomb interaction $W$ of the $GW$ approach should in principle be included and is expected to occur only in the limit $\mathbf{q} \to 0$ and for frequencies well below the gap. This effect has been proposed by Botti and Marques [PRL,**110**, 226404(2013)] to be important for large gap insulators with strong-LO-TO splitting. We have implemented this effect in the QSGW approach using a muffin-tin-orbital basis set, for crystals of arbitrary symmetry. The $\mathbf{q} \to 0$ contribution to the self-energy requires a careful treatment because of the integrable divergence of the Coulomb interaction, which is here done by means of the offset-$\Gamma$ approach. In the limit $\mathbf{q} \to 0$, the ratio of the total (lattice + electronic) macroscopic dielectric constant to the electronic contribution only can be represented by a generalized Lyddane-Sachs-Teller relation. We will discuss results for ionic crystals, like MgO, NaCl, and others with large LO-TO splittings $SrTiO_3$ and $V_2O_5$. We find the effect to be somewhat smaller than previously proposed and sensitive to the q-point sampling. The question to be addressed is how fast this effect decays as function of $q$ near $q = 0$.

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