

$\epsilon_{\text{OCL}} = \epsilon_g^{\text{qp}} - \epsilon_g$ calculated by OCL via local density approximation (LDA) (diamonds) is almost entirely due to the classical polarization energy Σ_{pol} (solid line) for the full range of sizes. Consequently, the fact that the quasiparticle gap ϵ_g^{qp} is different from the single-particle gap ϵ_g does not constitute a criticism of the latter, as OCL argue, but is merely a comparison of physically distinct quantities.

While OCL included surface polarization effects in the calculation of ϵ_g^{qp} , they neglected them in the calculation of the optical gap ϵ_g^{op} . Indeed, the total electron-hole interaction energy is $E_{\text{Co-1}}^{\text{eh}} + E_{\text{pol}}^{\text{eh}}$, where $E_{\text{pol}}^{\text{eh}} \simeq (e^2/R)(1/\epsilon_0 - 1/\epsilon_{\text{in}})$ describes the interaction between the electron and the surface polarization charge produced by the hole, and between the hole and the surface polarization charge produced by the electron [2,3]. Conventional dielectric functions, such as the one used by OCL, do not