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Optical absorption spectrum of $Ce@C_{82}$[1] ZHIFAN CHEN, ALFRED Z. MSEZANE, Clark Atlanta University — Optical absorption spectrum for the $Ce@C_{82}$ endohedral fullerene has been studied using the density-functional theory and the many-body Green's-function approaches. Geometry optimization was performed using the $DMol_3$software. A plane wave approach as implemented in the ABINITPackage has been used to solve the Kohn-Sham equation. Self-energy was evaluated by the GW approximation, which is the product of one-electron Green's function G_0 and screened Coulomb interaction W_0. Finally the optical absorption spectra have been calculated using the random phase approximation (RPA), RPA plus self-energy correction (RPA-GW) and the Bethe-Salpeter equation (BSE-GW).

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