Prediction of optical properties of gold nanoparticle with polymer brush

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In this paper, we predict the optical characteristics of monomer and dimer of quantum size gold nanoparticle with polymer (PEG & PMMA) coated core/shell hybrid structure through discrete dipole approximation (DDA) method. Also, we consider intrinsic size effect and non-local effect in gold nanoparticle@polymer core/shell. Through this system, we can find what roles of polymer shell are in their optical properties and how these quantum effects affect optical properties. The gold nanoparticle core size and polymer shell thickness are obtained by self-assembly gold nanoparticle@polymer core/shell which is simulated by dissipative particle dynamics (DPD) simulation. We found polymer shell depletes absorption cross section (Cabs(gold core)=Qabs(gold@polymer core/shell) Rgold core²), broadens full width at half maximum (FWHM) and LSPR peak goes red shift. There is no effect according to change of polymer shell 'composition, but the thickness of polymer shell is significant factor in optical properties. Generally, intrinsic size and non-local effect are occurred in Rgold nanoparticle < 10nm. Appling these effects to gold nanoparticle with polymer core/shell, intrinsic size effect decreases intensity of absorption peak but broadens FWHM. Non-local effect makes blue shift of LSPR peak. These effects can change the region of gold@polymer core/shell hybrid structure application.