Evolution of gold nanoparticle light absorption during agglomeration

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Gold nanoparticles are very attractive for biomedical applications due to their enhanced light absorption by collective oscillations of their surface electrons at the surface plasmon resonance wavelength, λ_{SPR} [1]. For example, their high λ_{SPR} sensitivity on the refractive index of the medium shows great potential for detection of small organic molecules and proteins [2]. The λ_{SPR} shifts from the visible light range (e.g. 530 nm) for single spheres to the near infrared spectrum (e.g. 780 nm) for non-spherical particles, such as nanorods. The λ_{SPR} sensitivity to refractive index of the medium also increases as with decreasing particle sphericity, ranging from 44 nm per refractive index unit (RIU) for single spheres to 224 nm/RIU for rods [3].

Here, discrete element modeling (DEM) is coupled with discrete dipole approximation (DDA) [4] to investigate numerically the evolution of gold light absorption during nanoparticle agglomeration. The DDA model is validated against simulations and experiments for single spheres and nanorods [5]. The DEM-derived agglomerate sphericity is quantified by the fractal dimension, D_f, evolving from 3 for single spheres to 1.91 for ramified agglomerates having more than 15 monomers. The gold λ_{SPR} shifts from 530 to about 650 nm during agglomeration due to plasmonic coupling effects [6], in good agreement with data [7]. The evolution of λ_{SPR} sensitivity to the medium is elucidated as a function of agglomerate size and benchmarked against those of single spheres and rods [3].

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