Kinetics of gold nanoparticle aggregation: Experiments and modeling

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We investigate the aggregation kinetics of gold nanoparticles using both experimental techniques (i.e., quasi-elastic light scattering, UV-visible spectroscopy, and transmission electron microscopy) and mathematical modeling (i.e., constant-number Monte Carlo). Aggregation of gold nanoparticles is induced by replacing the surface citrate groups with benzyl mercaptan. We show that the experimental results can be well described by the model in which interparticle interactions are described by the classical DLVO theory. We find that final gold nanoparticle aggregates have a fractal structure with a mass fractal dimension of 2.1–2.2. Aggregation of approximately 11 initial gold nanoparticles appears to be responsible for the initial color change of suspension. This kinetic study can be used to predict the time required for the initial color change of a gold nanoparticle suspension and should provide insights into the design and optimization of colorimetric sensors that utilize aggregation of gold nanoparticles.