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Title: Modelling of Role of Kinetics and Thermodynamics in Determining the Nanomorphology of Gold

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Nanoparticles offer a range of desirable properties that are intrinsically linked to their size, shape, and surrounding environment. Structure/property relationships used to describe these features are typically based on thermodynamic predictions of structure, but there are numerous experimental observations in the literature that do not conform to such predictions. For example, although the nanoscale phase diagram of gold indicates that icosahedral nanoparticles should only be expected at small sizes and low temperatures, they are persistently seen at larger sizes (and higher temperatures) with great frequency. These inconsistencies are routinely attributed to dominant kinetic influences, but this is rarely verified, since testing this hypothesis remains challenging and using conventional experimental or computational techniques. Therefore, in this presentation a new shape-dependent kinetic theory of nanomorphology is used to model the evolution of facetted gold nanoparticles, and to explore the edifying relationship between growth kinetics and thermodynamic stability. The kinetic results have been directly linked with the complementary thermodynamic model used to generate the nanoscale phase diagram, and the physical origins of observed shapes are explained. This study reveals that the frequent observation of icosahedral nanoparticles at thermodynamically-forbidden sizes is due entirely to their superior rate of coarsening, but that the observation of alternative shapes is due to a combination of influences that changes with size.