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Effective Reaction Coordinates in Competitive Nucleation of Gold Nanoclusters[1] CLETUS ASUQUO, RICHARD BOWLES, Dept. Chemistry, University of Saskatchewan — Many materials exhibit crystal polymorphism such that they can freeze to form a variety of different structures under the same conditions. Which structure is formed, and how, is determined by the nucleation kinetics that involves the creation of a critical embryo for the new phase. In classical nucleation theory, the embryo size is usually used as the sole order parameter to describe the reaction coordinate, but this does not always contain sufficient information to describe the formation of the different phases observed in a competitive nucleation process. We present an extension of the transition path sampling algorithm to the sampling of transition paths in a competitive process, as well as the development of a multiple paths maximum likelihood analysis used to obtain accurate reaction coordinates for the different transitions. The new techniques are used to study competitive nucleation in gold nanoclusters where non-crystalline structures such as icosahedra, decahedra and face-centered cubic crystals can form. The reaction coordinates, and analyses of the nucleation pathways, give new insights to how correlated local structures arrange to form more complex structures on longer length scales. In particular, we show that the formation of the tetrahedral subunits are important

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