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A Study of Energetics and Molecular Dynamic Simulations of Ag Nanoclusters MELIHAT MADRAN, MINE KONUK, Istanbul Technical University, SONDAN DURUKANOGLU, Sabanci University — We present results of molecular static and molecular dynamic calculations for the energetics of adatom and small cluster dynamics on the facets of truncated octahedral silver nano-particles. To identify the governing diffusion mechanisms during growth of the cluster the diffusion barriers on the various facets are calculated using nudged elastic band method based on the potentials extracted from embedded atom method. We also performed calculations to examine the possible influence of geometry on the diffusion dynamics of a single atom or a cluster on the facets of the nano-particles. Our growth simulations show that the energy barriers for diffusions between the different facets of truncated octahedral of silver remarkably reduced in the presence of the small aggregates on the facets. Using the results of energetic calculations and molecular dynamic simulations we further discuss the possible mechanisms for structural transition in a growth on truncated octahedral silver nano-particles. This work is supported by TUBITAK under Grand no. TBAG-109T105.

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