Supporting Information

Abnormal change of melting points of gold nanoparticles confined between two-layer graphene nanosheets

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1. Details of MD simulations

The phase transition of Au_N (n=1995-25536) nanoparticles confined between two-layer GNSs are investigated based on MD simulations. The length and width of a graphene nanosheet are 234.35Å and 238.62Å, respectively. The periodic boundary conditions are applied along x and z axes. Each of gold clusters is confined between two-layer GNSs. For simplicity, the systems studied are marked as Au_N-GNS, where N represents the number of gold atoms.

The EAM potential,[1,2] an *n*-body potential, has been widely developed for fcc metals by fitting experimental parameters,[3-5] which is confirmed to reproduce both surface properties and bulk of transition metals.[6] Therefore, the gold-gold interactions are described by the EAM potential.[3] Au-Au interaction energy, $E_{Au\text{-}Au}$, can be expressed by

$$E_{Au-au} = \sum_i F_i\left(\rho_{h,i}\right) + \frac{1}{2} \sum_i \sum_{j \neq i} \varphi_{ij}\left(r_{ij}\right) \tag{1}$$

where $F_i(\rho_i)$ is the embedding energy of atom i, $\rho_{h,i}$ is the host electron density at atom i generated by the surrounding atoms, $\varphi_{ij}(r_{ij})$ represents a short-range electrostatic interaction between atoms i and j, r_{ij} is the distance between atomic cores, and the sums are over all atoms. In current MD simulations. GNS is approximately considered as rigid superstructures of fixed atoms, which is similar to those in previous references.[7-9] The gold-GNS interactions are represented by a Lennard-Jones (L-J) potential. The relevant L-J parameters will be given latter.

During phase transition processes of the systems studied, each confined gold nanoparticle is melted by bringing it to a temperature above 1600K

for 1ns. Then, slow cooling run is carried out from 1600K to 300K with the temperature increments of 50K (for 1600-1350K and 850-300K) and 20K (for 880-1300K). The time step is set as 4fs. At each temperature, each system is first simulated at constant temperature (NVT ensemble) for 0.4ns and then simulated at constant energy (NVE ensemble) for 0.2ns. Finally, the slow heating run is performed on each system with same time step and temperature increment.

2. Supplementary figures

Fig. S1
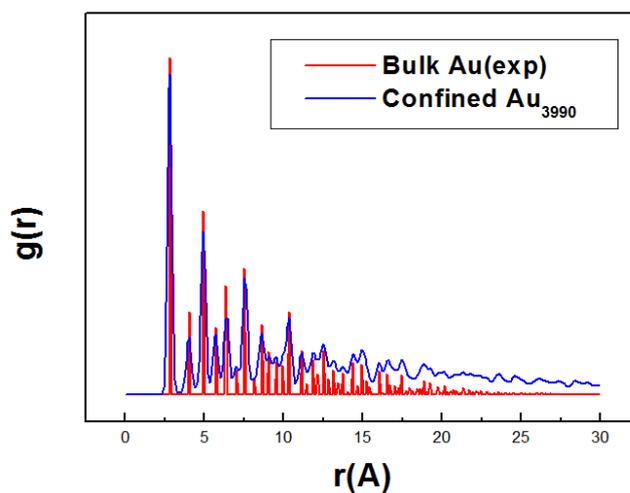
Fig. S1 The pair correlation function for experimental bulk gold and confined Au_{3990} nanoparticle.

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