Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

Intrinsic nano-transformation of Al_{55} clusters below the melting temperature JOONGOO KANG, SU-HUAI WEI, National Renewable Energy Laboratory, YONG-HYUN KIM, Korea Advanced Institute of Science and Technology — A recent series of experiments [1] have shown diverse melting behaviors in size-selected Al nanoclusters (Al_n). In particular, Al_{55} is a magic cluster that serves as a boundary for abrupt change of melting points when n is around 55. Here, resulting from first-principles molecular dynamics simulations of Al_{55} clusters, we reveal a new dynamic melting state that has both solid and liquid characteristics. In thermal fluctuations near the melting point, the low-energy tetrahedral Al_{55} survives through rapid, collective surface transformations — such as parity conversions and intervened row hopping — without losing its structural orders. The emergence of the collective motions is due to efficient thermal excitation of soft phonon modes at nanoscale. A series of spontaneous surface reconfigurations result in a mixture or effective flow of surface atoms as is random color shuffling of a Rubik's cube. This novel "lattice-liquid" state will provide useful insights into understanding stability and functionality of nano systems near or below melting temperatures. [1] G. A. Breaux et al., Phys. Rev. Lett. **94**, 173401 (2005).

Joongoo Kang
National Renewable Energy Laboratory

Date submitted: 19 Nov 2009 Electronic form version 1.4