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Origin of the Diverse Melting Behaviors of Aluminum Nanoclusters with Around 55 Atoms[1] JOONGOO KANG, SU-HUAI WEI, National Renewable Energy Laboratory, YONG-HYUN KIM, Korea Advanced Institute of Science and Technology — Microscopic understanding of thermal behaviors of metal nanoparticles is important for nanoscale catalysis and thermal energy storage applications. Using first-principles molecular dynamics simulations, we reveal the microscopic origin of the diverse melting behaviors of Al_N clusters with N around 55 [1,2]. The conceptual link between the degree of symmetry (e.g., T_d, D_{2d} and C_s) and solidity of atomic clusters is quantitatively demonstrated through the analysis of the configuration entropy. The size-dependent, diverse melting behaviors of Al clusters originate from the reduced symmetry ($T_d \rightarrow D_{2d} \rightarrow Cs$) with increasing the cluster size. In particular, the sudden drop of the melting temperature and appearance of the dip at N = 56 are due to the T_d-to-D_{2d} symmetry change, triggered by the surface saturation of the tetrahedral Al_{55} with the T_d symmetry.

[1] G. A. Breaux, C. M. Neal, B. Cao, and M. F. Jarrold, Phys. Rev. Lett. **94**, 173401 (2005).
[2] J. Kang, S.-H. Wei, and Y.-H. Kim, J. Am. Chem. Soc. (in press).

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