Atomic scale study of Al clustering and particle growth

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Recent years, aluminium nanoparticles has attracted many attentions for a variety of applications, such as propellant [1], high capacity hydrogen storage materials [2], nanocomposite materials [3], and biomolecules detection [4]. The nanoparticle dimensions can be an important factor for a given application as the mechanical and electrical properties of a material is particle size related. While the real-time growing process is normally difficult to be observed directly, theoretical study becomes essential to provide a better understanding of particle growth kinetics and mechanisms. We are investigating Al clustering and Al particle formation by using Molecular Dynamic (MD) simulation based on empirical potential. Trajectory calculations were performed to predict rate constant of association reactions of Al clusters. We will also discuss the important parameters (such as temperature, cluster size, etc) which effect on reaction kinetics.

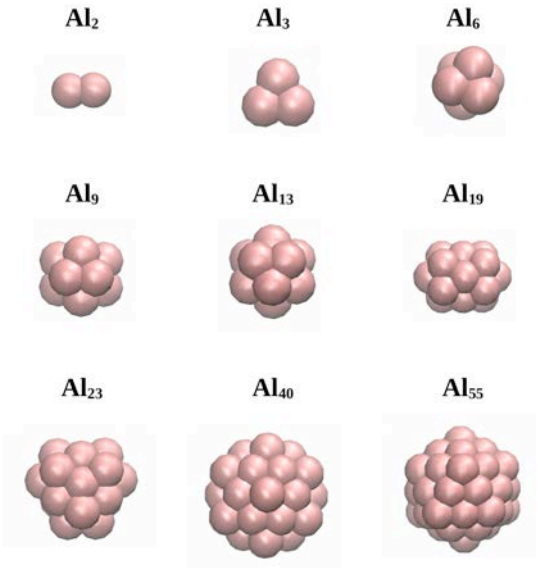

Figure 1. Visualization of geometry optimized aluminium clusters. It demonstrates global minimum configurations of involved Al clusters in this study.

1. References

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