Nanoscale Science in the Truhlar Group

Developing new semiempirical and multi-level / multi-scale methods for simulating nanoparticle growth and dynamics

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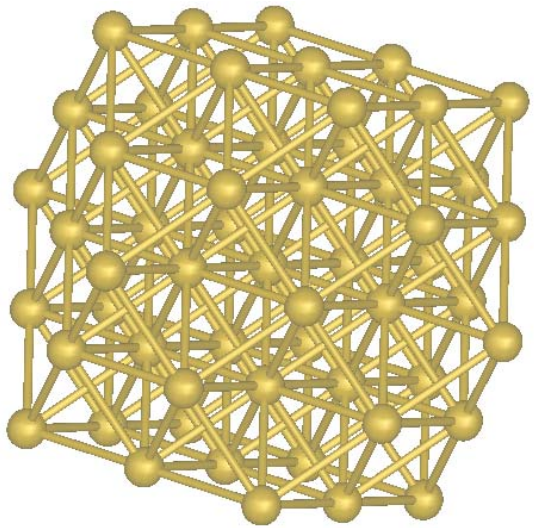

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New Semiempirical Methods for Nanoscale Systems

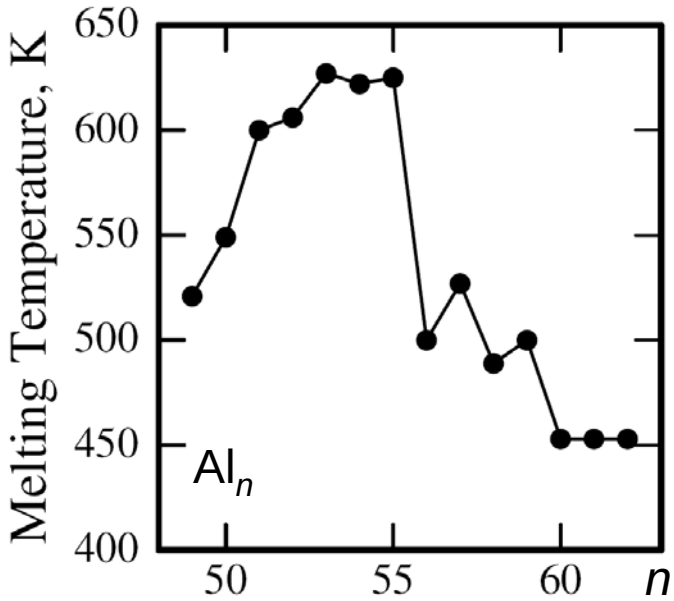
- In order to study properties of nanoparticles, need suitable model (potential energy function)
- Density functional theory often too expensive
- Analytical potential energy functions (PEFs, a.k.a. force field models) cost efficient but not always sufficiently accurate
- Tight binding more accurate than PEFs, cheaper than DFT, but has problems, e.g., with electrostatics

One possible solution: **Tight Binding-Configuration Interaction (TBCI)**

- Combination of two methods
  - Use tight binding orbitals
    - Semi-empirical approximation to solving the Schrödinger equation
  - Apply a configuration interaction (CI) treatment to the orbitals
- Non-iterative, accurate, and cost effective method to model aluminum nanoparticles

Simulation of Aluminum Nanoparticles

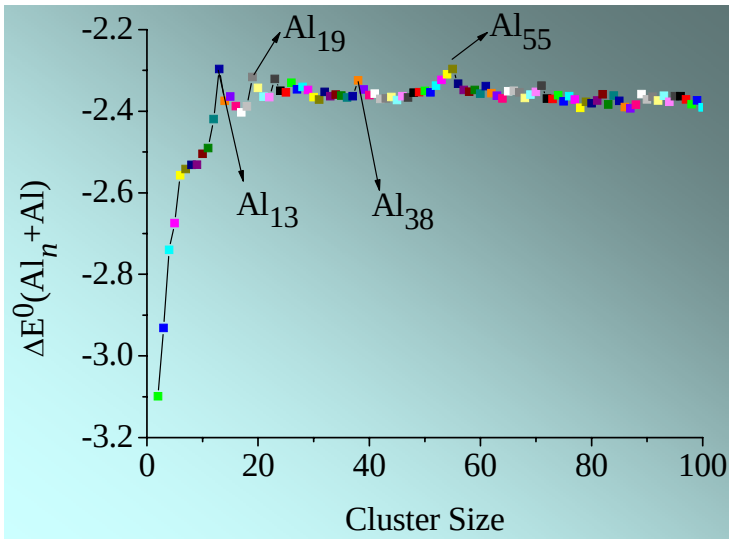
Aluminum nanoparticles can increase the burning rate of rocket propellants.



Melting

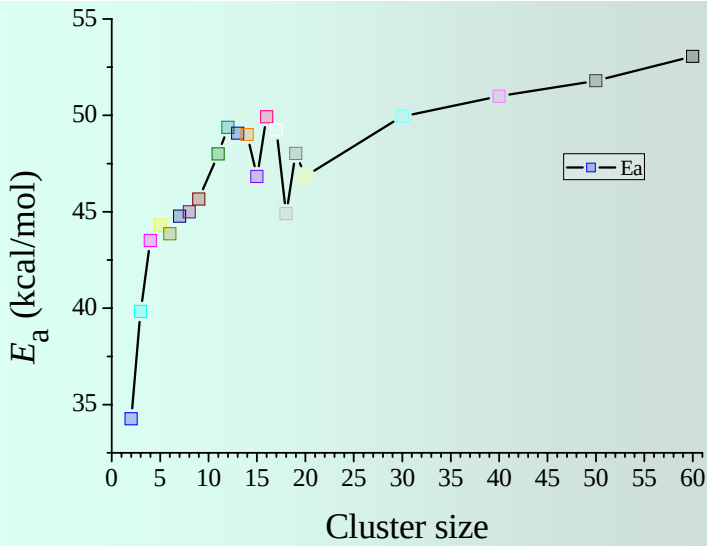
Properties of aluminum nanoparticles depend strongly on size.

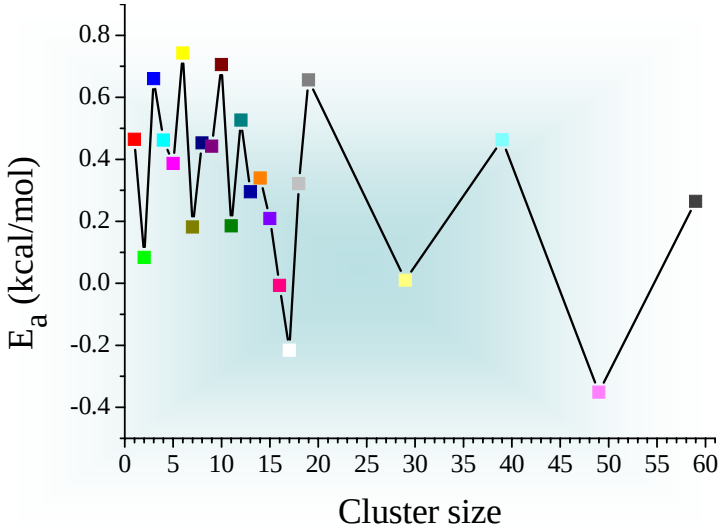
Stability



Magic numbers: 13, 19, 38, 55…

Aim: Better understanding of the size dependence of Al nanoparticle properties

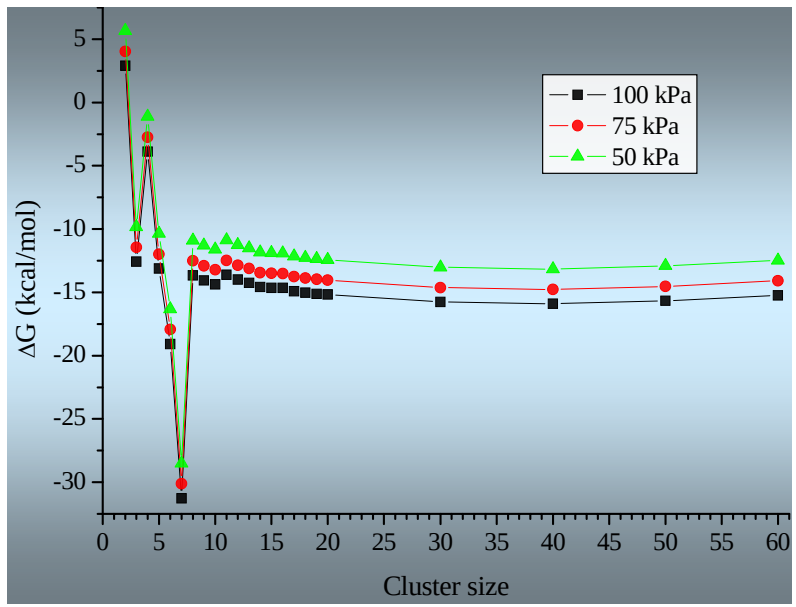




Activation energy of the $Al_n + Al \rightarrow Al_{n+1}$ reaction

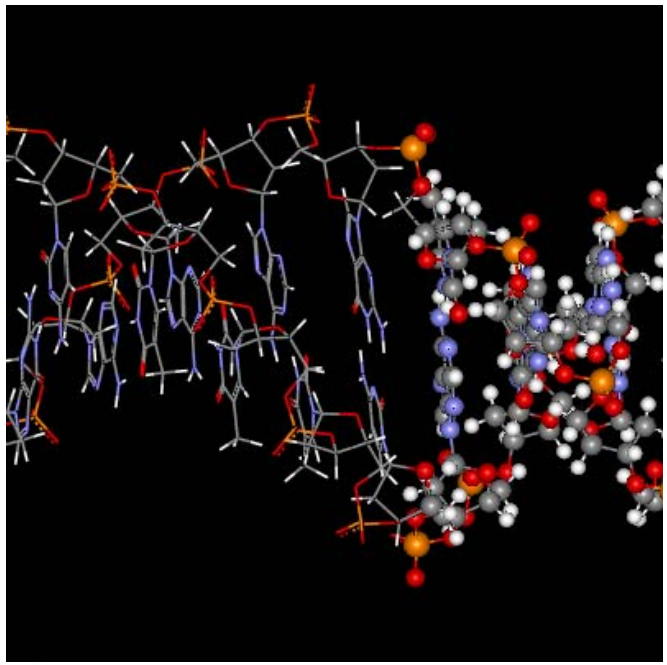
Activation energy of the $Al_n \rightarrow Al_{n-1} + Al$ reaction

Free energy change (kcal/mol) at 2000 K for adding one Al atom to an Al_n cluster



Adaptive Partitioning in Multilevel and Multiscale Simulations

We have developed an algorithm that enables the use of multilevel and multiscale simulation methods for systems where the **active region** is **not localized** and atoms enter and leave the active region during the simulation.



Examples include:

- Ligand exchange in solution
- Crack propagation in a material
- Diffusion and reaction on nanoparticles

⇒ **Can study larger systems over longer time scales without loss of accuracy!**