

Thermodynamics of free, supported and impurity doped clusters.

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Abstract

Clusters are known to display interesting properties which can be quite different from either bulk or single atom. Recently there has been considerable interest in finite temperature behaviour of clusters, especially in melting phenomenon. We examine a number of issues such as correlation between geometry and melting behaviour, effect of impurity on melting temperature and shapes of the heat capacities, and possible glassy behaviour of some clusters. We present our understanding of some of these issues, based on our density functional molecular dynamics work over the past several years. We will present our recent work on impurity (Silicon) induced effects on Ga₃₀. We will present some evidence for glassy behaviour in model as well as real clusters.

We examine evolutionary characteristics of shapes of Na clusters from N=8 to N=138. We establish a strong correlation between the symmetry (order and disorder), the closed shell nature and the melting temperature. We discuss examples of melting of Gold clusters (N= 20 and N=19). We demonstrate that it is possible to change the melting temperature and the shape of the specific heat curves by suitable doping of dilute impurities. Finally we will present evidence for glassy dynamics of Binary Lennard – Jones clusters¹.

¹ Work done in collaboration with group of S. Goedecker.