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Microcanonical molecular dynamics and histogram technique for drawing thermodynamics parameters of metallic clusters

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Temperature effects cause significant changes in the stability, structure and physical properties of finite system compared to the bulk. Therefore understanding the temperature effect is essential for any technological application. The fundamental quantity for studying the thermodynamics of a finite system is the classical density of states, Ω (E). Apart from the electronic properties obtained from electronic structure calculations, thermodynamic properties of clusters are mainly investigated by applying either the Monte Carlo techniques including the Simulated Annealing (MCSA) or constant temperature molecular dynamics techniques (NVT ensembles). In comparison on these methods, electronic structure calculation is a challenging task for transition metal system due to the complexity of their potential energy landscape and the complexity increases further in bimetallic alloys. Similarly, considering the Monte Carlo method and constant temperature MD simulations, calculation involves in the constant temperature despite the fact that an isolated cluster evolves at constant energy. Instead, the microcanonical ensemble (NVE ensemble) version of histogram method for determining densities of states or partition functions can be used to calculate the thermodynamic quantities, especially the heat capacity, Helmholtz free energy change and then the melting points of clusters.

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