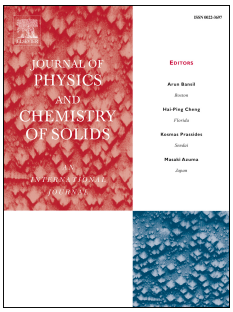
Accepted Manuscript



Size- and shape-dependent surface thermodynamic properties of nanocrystals

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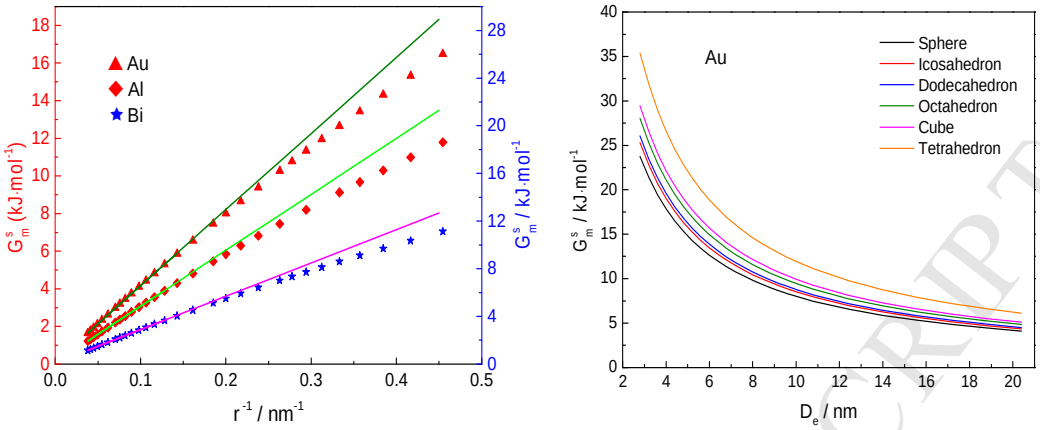
Graphical Abstract



By introducing interface variables into the Gibbs energy and combining Young-Laplace equation, relations between the surface thermodynamic properties (surface Gibbs energy, surface enthalpy, surface entropy, surface energy and surface heat capacity), respectively, and size of nanocrystals with different shapes were derived. Theoretical calculations of surface thermodynamic properties of Au, Al and Bi nanocrystals suggest that when r > 10 nm, the surface thermodynamic properties linearly vary with inverse particle size, and when r < 10 nm, the effect of particle size on the surface thermodynamic properties deviates from linear variation. For nanocrystals with identical equivalent diameter, the more the shape deviates from sphere, the larger the surface thermodynamic properties (absolute value) are.