Materials Science and Technology Division

"Predictive Modeling of Novel Structures and Structural Phase Transitions in Zero and One Dimensions"

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11:00 a.m.
4515/HTML, Room 265

Abstract:

Nanostructured materials usually have different physical properties from their bulk phases and show strong dependence on size with well-defined scaling behavior. However, when the sizes become too small, deviations from such scaling properties may emerge, as illustrated in the present talk using a few intriguing examples of metal nanoclusters and nanowires. We show, based on first-principles calculations, that strong relativistic effects can make gold clusters to be cage-like, which is non-compact and similar to C_{60}. Strong magnetic interaction can enhance the stability of layer-like structure of small Co clusters, similar to the fragment of bulk phase. For nanowires, we show how the size effect will lead to a peculiar cross-section that is in contrast with the prediction of the classic Wulff plot. I will also present examples illustrating how hydrostatic pressure induces structural transitions in nanoclusters and carbon nanotubes.

Host: Zhenyu Zhang