Heat Capacity and Thermal conductivity of Ge nanocrystals
SHANG-FEN REN, Illinois State University, WEI CHENG, Beijing Normal University, PETER Y. YU, University of California, Berkeley, and Lawrence Berkeley National Laboratory — Thermal conductivity of semiconductor materials has attracted a renewed research interest in recent years especially because the potential applications of nanocrystals and nanowires in thermoelectrics. By using an atomistic model we have investigated phonon properties in Ge and other nanocrystals. In the present work, we have extended our model to compute the heat capacities and thermal conductivities of Ge nanocrystals. The thermal conductivity has been calculated both by the classical Boltzmann approach and by a quantum mechanical approach along the lines of the quantized thermal conductance in 1D systems. The results of the two approaches are compared as a function of nanocrystal size and sample temperature.

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