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Zero-point motion and temperature effects on the band gap of semiconductor nanoclusters GABRIEL BESTER, P. HAN, Max-Planck-Institut für Festkörperforschung, Heisenbergstraße 1, 70569 Stuttgart, Germany — We calculate the band gap renormalization of semiconductor nanoclusters, avoiding the large computational costs associated with the calculations of the self-energy (Fan) and the Debye-Waller terms. This approach allows us to address clusters with a few hundred atoms. For Silicon nanoclusters, we obtain a band gap reduction of hundreds of of meV associated with the quantum zero point motion. This reduction rapidly increases with decreasing cluster size. Based on the Bose-Einstein distribution, we further study the temperature dependence of the band gap in semiconductor nanoclusters and find a band gap shift of -580 meV and -270 meV when going from T=0 to room temperature for silicon clusters with radius of 9.6 and 11.9 Å, respectively. Furthermore, we find that the band gap renormalization of semiconductor nanoclusters is dominated by the optic-like vibrational modes with Γ_4 point group symmetry.

G. Bester
Max-Planck-Institut für Festkörperforschung,
Heisenbergstraße 1, 70569 Stuttgart, Germany

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