MOMENTS-BASED TIGHT-BINDING CALCULATIONS OF LOCAL ELECTRONIC STRUCTURE IN INAS/GAAS QUANTUM DOTS

Harley T. Johnson
Dept. of Mechanical and Industrial Engineering, UIUC
362b Mechanical Engineering Building
1206 West Green Street
Urbana, IL 61801
htj@uiuc.edu

An order (N) tight-binding method is used to study electronic properties of realistic InAs quantum dots embedded in GaAs, with an emphasis on comparison to experimental scanning tunneling microscopy results. The approach is based on the method of moments, which is used to construct the local density of states approximately from a statistical sampling of the local atomistic structure around a particular point in the material. Moments of the density of states are built from products of the tight-binding hopping integrals connected neighboring atoms and orbitals; the parameterization used here is an sp3d5s* model. A combined maximum entropy method and kernel polynomial method is used to infer the density of states from moments obtained in this way. The method is ideally suited for comparison to high resolution local electronic structure measurements done using cross-sectional scanning tunneling microscopy (STM). Calculations are done to show the effects of free surfaces and strain relaxation. Quantum confinement in InAs quantum dots is shown directly by probing local densities of states at various atoms in and around the quantum dots. Using this computational probe method, the relationship between bandgap and quantum dot size is reduced to a simple equation. Finally, the method is directly applied to quantum dot structures studied experimentally using STM. The effects of disorder and atomistic features of the quantum dot matrix interface are studied directly using the moments-based tight-binding method.

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