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Large-scale Atomic Effective Pseudopotential Method for the Electronic Structure of Semiconductor Nanostructures GABRIEL BESTER, R. CARDENAS, F. ZIRKELBACH, P.-Y. PRODHOMME, P. HAN, R. CHERIAN, Max-Planck-Institut für Festkörperforschung, Heisenbergstr. 1, D-70569 Stuttgart, Germany — In the *Large-scale Atomic Effective Pseudopotential Method*, the Schrödinger equation of an electronic system is solved within an effective single-particle approach. *Atomic Effective Pseudopotentials* are utilized, which are derived from screened local effective crystal potentials obtained from self-consistent density functional theory calculations on elongated and slightly deformed bulk structures. A self-consistency cycle is not required, which reduces the computational effort. Furthermore, iterative solvers can be used to focus only on a few eigenstates of interest, e.g., states in the vicinity of the band gap of a semiconductor. Hence, this approach is particularly well suited for first-principles investigations of the electronic structure of nanostructures consisting of up to ten thousands of atoms, when the knowledge of the total energy of the system is not required. The treatment includes semi-local pseudopotentials (Kleinman Bylander separable form in real space) as well as the spin-orbit interaction. The obtained single-particle wavefunctions are then used to treat excited state properties by means of a configuration interaction approach. We will illustrate the capabilities of the method on some selected semiconductor nanostructures.

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

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