QuantumATK: An integrated platform of electronic and atomic-scale modelling tools - DTU Orbit (22/10/2019)

QuantumATK: An integrated platform of electronic and atomic-scale modelling tools
QuantumATK is an integrated set of atomic-scale modelling tools developed since 2003 by professional software engineers in collaboration with academic researchers. While different aspects and individual modules of the platform have been previously presented, the purpose of this paper is to give a general overview of the platform. The QuantumATK simulation engines enable electronic-structure calculations using density functional theory or tight-binding model Hamiltonians, and also offers bonded or reactive empirical force fields in many different parametrizations. Density functional theory is implemented using either a plane-wave basis or expansion of electronic states in a linear combination of atomic orbitals. The platform includes a long list of advanced modules, including Green's-function methods for electron transport simulations and surface calculations, first-principles electron-phonon and electron-photon couplings, simulation of atomic-scale heat transport, ion dynamics, spintronics, optical properties of materials, static polarization, and more. Seamless integration of the different simulation engines into a common platform allows for easy combination of different simulation methods into complex workflows. Besides giving a general overview and presenting a number of implementation details; not previously published, we also present four different application examples. These are calculations of the phonon-limited mobility of Cu, Ag and Au, electron transport in a gated 2D device, multi-model simulation of lithium ion drift through a battery cathode in an external electric field, and electronic-structure calculations of the composition-dependent band gap of SiGe alloys.

General information
Publication status: Published
Organisations: Department of Physics, Center for Nanostructured Graphene, Synopsys Denmark ApS
Corresponding author: Smidstrup, S.
Number of pages: 36
Publication date: 2020
Peer-reviewed: Yes

Publication information
Journal: Journal of Physics: Condensed Matter
Volume: 32
Article number: 015901
ISSN (Print): 0953-8984
Ratings:
BFI (2020): BFI-level 1
Web of Science (2020): Indexed yes
Original language: English
Keywords: Atomic-scale modelling, Density functional theory, Semi-empirical methods, Tight-binding, Force fields, First-principles simulations, Non-equilibrium Green's function
DOIs: 10.1088/1361-648X/ab4007
Source: FindIt
Source ID: 2453318405
Research output: Contribution to journal > Journal article – Annual report year: 2020 > Research > peer-review