DEEPEN, kp-Metadata

Template for workflow modelling metadata

1. The properties and behaviour of a particular material (textual description).
2. Description of the chain of models calculating these properties and behaviour
   (each model identified as electronic, atomistic, mesoscopic or continuum and by reference to a Chapter in Review of Materials Modelling IV available on http://ec.europa.eu/research/industrial_technologies/e-library.cfm).
3. Publication documenting the workflow

1. **Generic physics of the model equation**
   k.p Effective Hamiltonian model (1.2.5 in RoMM)
   1.1. This is a materials model for electrons
   1.2. The model has a physics/chemistry equation:
   Time-Independent Multi-band Schrödinger Equation with physics quantities:
   wave functions, band structure parameters, electrostatic potential
   and closure relation for Hamiltonian that involve a :
   material-specific k.p parameters, including position-dependent band edge energies, spin-orbit coupling energies, crystal field splitting energies, band structure deformation potentials, strain tensor, polarization fields, k.p matrix elements, Number of treated conduction and valence bands
   1.3 Publication documenting the model
   The k.p Effective Hamiltonian is presented in detail in the text book "The k.p Method Electronic Properties of Semiconductors", Lok C. Lew Yan Voon and Morten Willatzen (Springer 2009). There is a good overview in Peter Y. Yu and Manuel Cardona. (2010). Fundamentals of Semiconductors: Physics and Material Properties. 4th ed. Heidelberg: Springer.

2. **End-user problem/system that is simulated (type of metadata: declarations)**
   This is the "model application", "case to be studied".
   2.1. Specify material properties, behaviour and/or material manufacturing processes simulated. (Describe the case textually as if you were going to calculate it analytically. Think of exercises you did in the physics lessons: example: a person on a ladder on a slippery floor).
   Calculation of electronic states in semiconductor nanostructures, to determine electron and hole confinement energies and wave functions in the nanostructure, taking account of influence of factors such as nanoparticle composition and geometry, as well as influence of externally applied perturbations such as electric and magnetic fields
   2.2. Size, form, geometry, picture of the system and time lapse of the process
   Unit Cell (Supercell; Simulation box)
   2.3. Physics metadata for system that is simulated. Here should be listed

- physics quantities that do not appear in the physics equation and not in the case description above but that are relevant to describe the system/problem/ model application/case like e.g. density, external pressure, viscosity, chemical composition, impurities, mobility
- process conditions (like heated walls, external pressures, bending forces) to be simulated),

(Note this should not describe the output!)

chemical composition, external stress and electrostatic potential

2.4 Publication documenting the simulated case

3. **Computational modelling metadata for the case that is simulated (type of metadata: values/data)**

3.1 Numerical Solver

3.2 Input you need to start computing, e.g. times step, number of "fictitious" particles (only in case this can be chosen freely like in Lagrangian solvers), grid size, computational boundary conditions, "fictitious" particle positions and velocities (that you can choose freely but are necessary to start computing).

- Choice of periodic or hard-wall boundary conditions
- Choice of finite-element, finite-difference or plane-wave calculation method
- Material composition as a function of position within supercell
- Choice of k-points for calculation

3.3 Initialisation of all quantities and parameters (appearing in Ch1, Ch2, Ch3.1): (these are the code's input files and can for the moment remain empty until uploaded into a repository)

3.4 Keywords describing "raw output" calculated by the model for the entities

Wavefunctions, single particle energies

3.5 Keywords for "post processed properties" calculated for finite volumes from the raw output calculated with <please describe the post processor>:

- single-particle carrier confinement energies and interband transition energies (directly from single particle energies)
- band structure [E(n,k)]
- density of states (DOS)
- transition matrix elements for optical recombination (calculated from wavefunctions)
- band dispersion for one-band models (directly from single particle energies in multi-band model)
- exciton and biexciton energies (based on calculations using configuration interaction model)
- ……

3.4 Margin of error of property calculated under 3.3

- Two sources of error: 1) convergence of calculation and 2) accuracy in materials parameters used;

- convergence typically to within 1 meV (best case) to 10 meV (worst case)
- error due to choice of materials parameters from ~1 meV (best case) to ~100 meV (extreme case)

3.4 Publication documenting the simulation