Template for workflow modelling metadata

1. The properties and behaviour of a particular material

   Doped organic semiconductors
   Current-voltage-luminance curves of OLEDS and OTFTs
   Doping efficiency and electrical conductivities of doped organic layers, accounting for the presence of impurities

2. Description of the chain of models calculating these properties and behaviour

   DFT, GW, BSE (electronic) (part of MESO-EL code)
   Micro-electrostatic model (electronic) (part of MESO-EL code)
   CG-MD (mesoscopic) (MESOMORPH code)
   Statistical mechanics solved by kinetic Monte Carlo (electronic) (MESOTRANS code)
   Drift Diffusion (continuum) (ATLAS code)
   ElectroMagnetic model (continuum) (ATLAS code)

3. Publication documenting the workflow

Metadata for a MESO-EL DFT part

1. **Generic physics of the model equation**

   DFT, GW, BSE electronic

   1.1. This is a materials model for electrons, holes and excitons

   1.2. The model has a

   - Physics/chemistry equation the Schroedinger equations that involve the following physics quantities: wave function, energy, Hamiltonian
   - Materials relation: pseudopotentials

   1.3 Publication documenting the above:

   http://bigdft.org/Wiki/index.php?title=BigDFT_website

2. **Case that is simulated**

   2.1. Material and and/or material manufacturing processes simulated

   Transfer (hopping) of electrons, holes and excitons in Organic Molecules and polymers, pristine and doped and the forces between atoms

   2.2. Application domain (size and form, geometry, picture of the domain)

   Molecules and, for polymers, conjugated segments

   2.3. Physics metadata for case that is simulated

   chemical composition, impurities, number of electrons

   2.4 Publication documenting the above: see 1.3

3. **Computational metadata for the case that is simulated**

   3.1 Input you need to start computing, *e.g. times step, number of "fictitious" particle, grid size, computational boundary conditions, "fictitious" particle positions and velocities (that you can choose freely but are necessary to start computing.*

   type of computational boundary conditions: periodic supercell

   3.1 Initialisation of quantities: these are the code's input files and can remain empty until uploaded to repository

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

   LUMO and HOMO orbitals.

   3.3 Keywords for "post processed properties" calculated for atoms in small molecules from the raw output calculated with <please describe the post processor>

   transfer integrals needed for hopping rates for MESO-TRANS and force fields for MESO-MORPH interface band offsets for MESO-TRANS and ATLAS

   3.4 Margin of error of property calculated under 3.3 10%

   3.4 Publication documenting the above: see 1.3

Metadata for a MESO-EL micro-electrostatic part

1. **Generic physics of the model equation**

Electrostatics

1.1. This is a materials model for electrons, holes

1.2. The model has as

- Physics/chemistry equation: Coulomb equation (First Maxwell equation) that involve physics quantities: charge distribution, electrostatic field, permittivity
- Materials relation: D=eps.E

1.3 Publication documenting the above P Friederich, F Symalla, V Meded, T Neumann, and W Wenzel *J. Chem. Theory Comput.*, 2014, 10 (9), pp 3720–3725

2. **Case that is simulated**

2.1 Material and/or material manufacturing processes simulated

The interaction between one or more charges localised on molecules or polymer segments and the surrounding electrostatic environment

Organic Molecules and polymers, pristine and doped,

Influence of electrostatics on electron and hole orbital energies

2.2 Application domain size and form (geometry, picture of the domain)

100-1000 molecules in disordered morphology

2.3 Physics metadata for case that is simulated

chemical structure of molecule/polymer

electronic structure calculated with many-body models (output form DFT)

Temperature, pressure

2.4 Publication documenting see 1.3

3. **Computational metadata for the case that is simulated**

3.1 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).,

computational boundary conditions: Periodic supercell

vacuum partial charges of molecules (approximation to electronic structure in 2.3)

3.2 Initialisation of quantities:

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

Electrostatic energies of groups of atoms

3.4 Keywords for "post processed properties" calculated for atoms in small molecules from the raw output calculated with <please describe the post processor>

Free energy difference contribution due to hopping (rates from Marcus theory calculated by MESO-EL DFT)

3.5 Margin of error of property calculated under 3.3 20%

3.6 Publication documenting see 1.3

Metadata for a MESO-MORPH

1. Generic physics of the model equation

CG-MD, mesoscopic

1.1 This is a materials model for beads representing molecules or for polymers, groups of monomers

1.2 The model has a

- physics/chemistry equation Newton Dynamics (classical equations of motion) with as physics quantities (parameters and variables that appear in these equations) force field, particle trajectories and velocities, temperature, pressure, particle locations, velocities
- closure relation a Force Field for interaction between beads derived from the electronic structure obtained in MESO-MORPH that depends on the atomistic structure of the groups of atoms that make up the beads.

1.3 Publication documenting the above

V. Lemaur, L. Muccioli, C. Zannoni, D. Beljonne, R. Lazzaroni, J. Cornil, Y. Olivier, *On the supramolecular packing of high electron mobility naphthalene diimide copolymers* Macromolecules, **46**, 8171-8178 (2013)

2. **Case that is simulated**

molecular organisation in OLEDS

2.1 Material and/or material manufacturing processes simulated

structural morphology for organic small molecules and polymer semiconductors for each device structure

2.2 Application domain (size and form, geometry, picture of the domain)

amorphous structure at high temperature and low density or ordered structure

Time lapse of the simulations: picoseconds

2.3 Physics metadata for case that is simulated

mass density, chemical composition and impurity profiles,

2.4 Publication documenting the above see 1.3

3. Computational metadata for the case that is simulated

3.1 Input you need to start computing, e.g. times step, number of "fictitious" particles

Timestep: Femtoseconds

Computational boundary conditions:

Periodic at constant pressure or constant volume

Positions and velocities for typically 10^4 to 10^5 particles

3.2 Initialisation of quantities:

initial positions of beads

3.2 Keywords describing "raw output" calculated by the model for the entitie

particle trajectories, velocities vs time averaged ~1000 timesteps after equilibration

2.3 Keywords for "post processed properties" calculated from the raw output

predictions of morphology for equilibrium or arrested morphologies

3.4 Margin of error of property calculated under 3.3 10%

3.5.Publication documenting the above see 1.3

Metadata for MESO-TRANS

1 Generic physics of the model equation

statistical mechanics BTE solved by kinetic Monte Carlo, electronic

1.1 This is a materials model for charge carriers: electrons, holes, singlet and triplet excitons

1.2 The model has a

- physics/chemistry equation BTE that involve physics quantities probability that a number of particles all occupy a very small region of space, the "force" term corresponds to the forces exerted on the particles by an external influence (not by the particles themselves), the "diff" term represents the diffusion of particles, and "coll" is the collision term - accounting for the forces acting between particles in collisions, pair correlation function,
- and a closure equation waiting times from site energies and transfer integrals, events for particles (hops, recombination, generation), interface band offsets

1.3 Publication documenting the above *Mesoscopic kinetic Monte Carlo modeling of organic photovoltaic device characteristics* R G E Kimber, E N Wright, S E J O'Kane, A B Walker, J C Blakesley Phys. Rev. B (2012) 86, 235206

2 Case that is simulated (end-user-type description)

2.1 Material properties and/or material manufacturing processes

Charge and energy transport in organic semiconductors in the ICT device layers

2.2 Application domain (size and form, geometry, picture of the domain)

ICT device architecture

and time lapse of the simulations: picoseconds-milliseconds

2.3 Physics metadata for case 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 application/case like e.g. density, external pressure, viscosity, chemical composition, impurities, mobility
- restrictions like e.g. physical boundary conditions, physical initial conditions

Mass density, chemical composition, impurity profiles

Particle locations (related to the above mentioned probability)

2.4 Publication documenting the above see 1.3

3. Computational metadata for the case that is simulated

3.1Type of input you need to start computing e.g. times step, number of “fictitious” particles

Boundary conditions For a stacked device, in direction parallel to the line joining the contacts, ohmic or Schottky boundary conditions, depending on the materials composition of the contacts and active layers adjacent to the contacts

In plane parallel to the contacts, periodic boundary conditions

For organic thin film transistors, boundary conditions depend on the geometry of the OTFT and will include ohmic or Schottky boundary conditions at each contact.

times step: N/A

number of particles: typically 10^4, depending on device

3.2 Initialisation of quantities:

initial positions of charges and excitons

3.2 Keywords describing “raw output” calculated by the model for the entities

Particle trajectories and currents averaged ~1000 runs

3.3 Keywords for “post processed properties” calculated for <entity: atoms, grains, finite volumes> from the raw output calculated with <please describe the post processor>

fluxes

3.4 Margin of error of property calculated under 3.3 5%

3.4 Publication documenting the above see 1.3

Metadata for a ATLAS DD part

1 Generic physics of the model equation

continuum CFD

1.1. This is a materials model for finite volumes in which the electrons are considered as a continuum

1.2. The model has

- physics equations for drift diffusion of electrons, holes and excitons that involve as physics quantities density, diffusivity, and concentration and
- closure relations relating diffusion coefficients and mobilities, and the first Maxwell law (Gauss' law) , relation between displacement and E field and relation between E field and potential that together give Poisson's equation that involve as physics quantities E field, displacement, charges, mobilities, diffusion coefficients, densities of states, band offsets

1.3 Publication documenting the above Silvaco website.

2 Case that is simulated (end-user-type description)

2.1 Material properties and/or material manufacturing processes simulated: diffusion in organic semiconductors

2.2 Application domain size and form (geometry, picture of the domain) device architecture,

and time lapse of the simulations milliseconds to seconds

charges injected at contacts

Bias voltage applied between contacts

2.3 Physics metadata for case that is simulated

charge mobilities, exciton diffusion coefficients, interface band offsets,

2.4 Publication documenting see 1.3

3. **Computational metadata for the case that is simulated**

Type of 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).

Type of boundary conditions: periodic in plane normal to contacts

For a stacked device, in direction parallel to the line joining the contacts, ohmic or Schottky boundary conditions, depending on the materials composition of the contacts and active layers adjacent to the contacts

In plane parallel to the contacts, periodic boundary conditions

For organic thin film transistors, boundary conditions depend on the geometry of the OTFT and will include ohmic or Schottky boundary conditions at each contact.

initial conditions: charge density profiles for the initial bias, often 0V

3.1 Initialisation of quantities:

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

Current-voltage curves
Doping efficiency and electrical conductivities of doped organic layers, accounting for the presence of impurities

3.3 Keywords for “post processed properties” calculated for finite volumes from the raw output calculated with <please describe the post processor>

Impedance spectra, Equivalent circuits

3.4 Margin of error of property calculated under 3.3 10%

3.4 Publication documenting see 1.3

Metadata for ATLAS ElectroMagnetics (optical)

1. Generic physics of the model equation

model type and name chosen from RoMM content list

Electromagnetic Maxwell equations

1.1. This is a materials model for finite volumes

1.2. The model has

- a physics/chemistry equation Maxwell's equations that involve physics quantities Electric field E, magnetic field H, electric flux density D, magnetic flux density B, current density, charge density, position and time
- and closure equation dependence of fluxes on fields (D on E and of B on H) that involve physics quantities: permittivity and permeability

1.3 Publication documenting Silvaco website.

2.Case that is simulated (end-user-type description)

light emission from OLEDs

2.1 Material and and/or material manufacturing processes simulated

Light emission from doped organic semiconductor in OLED

2.2 Application domain size and form (geometry, picture of the domain) and time lapse of the simulations

OLED consisting of stacked layers, micron dimensions x-y, 100 nm between contacts

2.3 Physics metadata for case 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 application/case like e.g. density, external pressure, viscosity, chemical composition, impurities, mobility

  Intensity profile and colour of emitted photons
- restrictions like e.g. physical boundary conditions, physical initial conditions (specifying the case to be simulated),

  Dirichlet or Neumann BCs depending on electrode configuration

2.4 Publication documenting the above: see 1.3

3. Computational metadata for the case that is simulated

3.1 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).

Grid size,

3.2 Initialisation of quantities: (these are the code's input files and can for the moment remain empty until uploaded into a repository)

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

Intensity profile and colour of emitted photons

3.4 Keywords for "post processed properties"

Luminance, colour profile

Current-voltage-luminance curves, emission colours

Doping efficiency and electrical conductivities of doped organic layers, accounting for the presence of impurities

3.4 Margin of error of property calculated under 3.3 1%

3.4 Publication documenting the above: see 1.3