D1.1

Report on use cases and system requirements

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Version	Date	Modified by	Modification reason
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v.02	30/07/2019	Arrigo Calzolari	Revision
v.03	29/06/2021	Matthias Büschelberger	Main revision of motivation and inclusion of user stories
v.04	15/07/2020	Arrigo Calzolari	Final revision

Contents

[1] Acronyms are marked in purple in the text and defined at the end of the document.

1. Executive Summary

The design foundations of the Interoperable Materials-To-Device (IM2D) simulation box are identified using the agile approach, and the registry of user story and application cases are described based on the data collected from the partners. The user stories are extended and the most important specifications to be implemented within the INTERSECT project context are established in terms of personas, features and corresponding user stories. This analysis is complemented by the European Materials Modeling Council (EMMC) Materials mOdelling metaDAta (MODA) workflow that exposes the most relevant elements involved in the modelling workflows and is used to guide in the development process, particularly in the ontology development (see deliverable D1.3).
Based on this analysis, a general view on the system requirements is also presented in terms of rational, risk and mitigation. In summary, the work is going on as planned, there are no major deviations. The results of this deliverable provide sound inputs for Tasks 1.2 and 1.3.
This amended version (M31) updates and complements the original file delivered at M6, and includes examples of the user stories for both the Material-to-Device (M2D) and the Device-to-Material (D2M) workflows.

2. Motivation and description of the work done

This deliverable addresses Task 1.1: Use cases and architecture.
The main goal of the INTERSECT project is the release of a software solution (IM2D) that allows industrial stakeholders to model, optimize and design new complex devices (such as memristors for synaptic electronics), by using automated and state-of-the-art codes for both the electronic/atomistic (DFT) characterization of the materials and the electrical response of the device. Interoperability is the key element we adopted to realize this objective, since it is the natural route of choice to allow different stakeholders to access technology, as well as to transfer and interpret concepts and data unambiguously. Two levels of interoperability are considered and implemented in this project:
Level I: **syntactic interoperability**, which provides the structural interconnection among physical models and codes, e.g., coupling-and-linking of models and the generation of a data pipeline between existing codes.
Level II: **semantic interoperability**, which provides the description of the information meaning in a formal, machine-readable, and processable way (metadata and schema based on semantics).
Syntactic interoperability involves the sharing of data among models/codes (simulation hub) and/or databases (data hub), and it is the necessary step for **automation**, data curation and traceability of the results. Rather, syntactic interoperability alone is not sufficient to reduce the

complexity of the problem and to make IM2D accessible to industrial users. As is - albeit automated - running the entire flow (materials and device cycles) would require the user to have advanced skills in several fields such as quantum physics and material science (materials simulation), informatics and electrical engineering (device modelling). This would be technically possible but practically unusual. In order to make IM2D a product that really can be exploited by industrial users, it is necessary to tailor the complexity of the input/output and of the workflows on the basis of the specific knowledge level of the user, letting all the rest automatically run in the backend. This calls for the implementation of a semantic interoperability level that generates an **interdependence between concepts and data**: concepts provide the meaning for a set of data, and data sets cannot be exchanged without a linking concept that describes their meaning.

IM2D provides a semantic interoperability level by analyzing the specific use cases from users, identifying data and information needed to be exchanged, and selecting the most appropriate workflows that will be operated by simulation codes in the backend through the syntactic layer (see Figure 1).

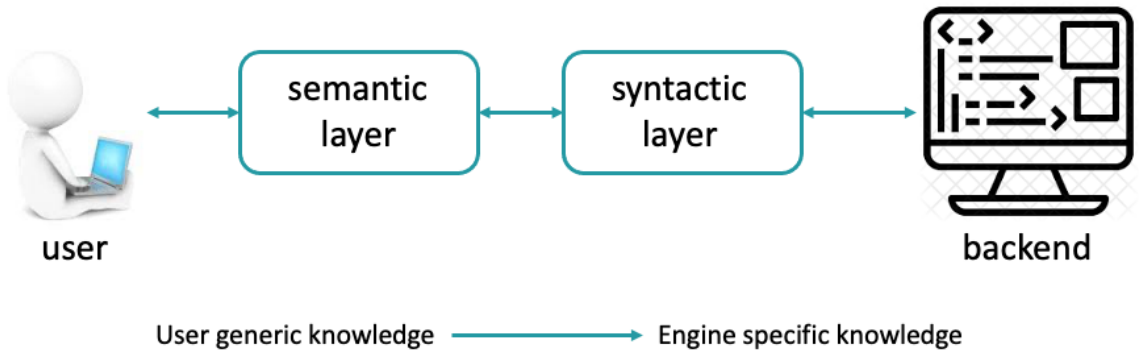


Figure 1 – Hierarchical interoperability levels.

The objective of Task 1.1 is to upscale the design foundations of the IM2D simulation box and to identify the most relevant parameters, physical models, codes, workflows, user profiles, and user stories necessary for the implementation of both the syntactic and semantic interoperability levels developed in WP2.

The first outcome of this task is a **registry of user story and application cases** that will be *continuously updated* (i.e., for completion of the requirements). The register allows us to identify reliable users' profiles (***persona***) and their level of knowledge, to which it corresponds a specific set of workflows and the access to specific data. For the two main operation modes proposed in the DoA, (i.e. M2D and D2M), we identified the physical properties that are entered as input in the materials (Density Functional Theory - DFT, Quantum ESPRESSO - QE and SIESTA) and device (Ginestra™) steps. The most important ones will be explicitly

implemented as “materials properties on demand” in WP2, and made automatically available to the entire IM2D through the AiiDA infrastructure.
All simulation models, relations and implementation solutions are formalized and standardized in terms of EMMC MODA schemes, as resulted by using the MODA online portal on https://emmc.info/moda to further guide the development process. This constitutes the formal foundation of the syntactic interoperability layer.
The second outcome of this task is a set of Extended User Application Cases Stories (EPICS), which are mandatory for the semantic interoperability level and for the implementation of the corresponding wrappers with the SimPhoNy infrastructure (WP2). The formal standardization of the physical quantities (materials entities, models, materials relations) and of the calculation types is based on an INTERSECT-specific extension of the European Materials Modelling Ontology (EMMO), which is the subject of deliverable D1.3.

3. Deviation from the work planned in the DoA

While this task is planned to end at M6, the DoA clearly mentioned that the user registry and stories shall be updated continuously. Nevertheless, these actions can move to Tasks 1.2 (ontology) and Task 1.3 (requirements) without loss of generality. This deliverable can be considered complete, while additional user stories and drill down of interoperability requirements, as well as updates on the requirements, can be done directly on the collaborative code repository where such relevant information on such development would best reside.

4. Results

4.1 Registry of user story and application cases

The registry of user cases and application cases has been collected from all partners involved in the task, and cover most of the use scenarios expected. These user stories have been extended to also include the type of ***persona***, using the system so as to be able to tailor the user interaction and requirements for the targeted users (*personas*). Hence, in addition to the DoA, a *persona* registry is created. Personas are then categorized according to expertise and know-how in modelling, in general and in device design and operation.
The user stories are focused on the *persona*, and on how they operate the IM2D within the context of an application. The applications are essentially EPICS that are user cases, i.e., what the user needs to achieve. A user story is essentially aimed at capturing the functionality of a software tool from the user perspective. The use case is part of the user story.

A user story has the following structure:

- As a <role/persona>, I want <feature> so that <reason>

The user case as defined in the DoA and in materials engineering applications is normally the "***feature***" and "***reason***" parts.

We start by defining the *persona* registry followed by the *features*, then the selected user stories are extended. Finally, MODA covering the modelling related to the most important user stories and applications are given.

4.1.1 Persona

The *persona* registry defines who will use the IM2D box. Within the context of INTERSECT, the following *personas* have been identified:

A. Engineer in a company (SME, or large enterprise)
   - **a. No experience/knowledge in materials modelling (process engineer)**
     1. but expert in electronic circuits and device optimisation
     2. **but expert in device optimisation only**
     3. but expert in electronic circuits optimisation only
   - **b. Has some experience/knowledge in materials modelling in general, mostly continuum**
     4. and expert in electronics circuits and device optimisation
     5. **and expert in device optimisation only**
     6. and expert in electronic circuits optimisation only
   - c. Has some experience in materials modelling in general including discrete atomistic and mesoscopic
     7. and expert in electronic circuits and device optimisation
     8. and expert in device optimisation only
     9. and expert in electronic circuits optimisation only
   - d. Has some experience/knowledge in materials modelling in general including electronic property models (e.g. density functional, etc)
     10. and expert in electronic circuits and device optimisation
     11. and expert in device optimisation only
     12. and expert in electronic circuits optimisation only

B. Researcher in academy (University or research lab)
   - a. Expert in device optimisation only
     13. theory and modelling of devices
     14. experimentalist (e.g. device fabrication and characterization)
   - b. Expert in circuits optimisation only
     15. theory and modelling of extended circuits

16. experimentalist (e.g. setup of architectures and networks)

c. **Expert in materials only**
    17. theory and modelling of materials
    18. experimentalist (e.g. material growth and characterization)
d. Students/in-training young scholars in
    19. theory and modelling of materials
    20. theory and modelling of devices
    21. growth and characterization of materials (experimentalist)
    22. fabrication and characterization of devices (experimentalist)

Prioritization: in INTERSECT, we have picked the following main three top priority *personas* on the basis of the market demands communicated by the industrial partners (software owners):

Persona #: 1 Process engineer in a company, expert in optimization/characterization of specific materials but with no experience/knowledge in device modelling (Aa2). This *persona* is the prototypical final user of IM2D as a black-simulation box. Participant people from the INTERSECT AMAT group are prototypes of this *persona*.

Persona #: 2 Engineer in a company, expert in the optimization/characterization of specific devices but with experience/knowledge in material (electronic/atomistic) models (Ab5). Participant people from the INTERSECT FMC/IMEC group are prototypes of this *persona*.

Persona #: 3 Researcher from academy, with background in materials modelling, including electronic models but with no experience/knowledge in device or circuit optimization (Bc17). Participant researchers from the INTERSECT CNR, EPFL, and ICN2 groups are prototypes of this *persona.*

4.1.2 Features

There are two main classes of features (in the agile sense defined above) and in accordance with the DoA:

1. **Material-to-device** (M2D): In this class of features, material properties, including structural and electrical effects of defects initially calculated by using electronic and discrete modelling, are further exploited by the Ginestra™ code within the IM2D framework to simulate the electrical response of a selected device.
2. **Device-to-material** (D2M): Specific electrical device characteristics (e.g., I-V curve) are interpreted by using the Ginestra™ code in the IM2D box to identify/determine specific material properties (e.g., spatial and energetic distribution of defects). Starting from the user's query, the interoperability Hub (iHub) launches a device simulation cycle that, exploiting specific datamining functionalities of Ginestra™, namely through *defect discovery tool*, extracts material and defect parameters (e.g., the bandgap,

defect energies, etc.) from the filtering of the electrical device characteristics. These material and defect parameters are used to activate a search in the database (AiiDA) and to launch a set of material cycles for the DFT-assisted identification of the target material and defect configurations. Device and material results (including stable defect configurations) are stored in the database as metadata, and passed as final user's output through the Graphical User Interface (GUI) interface.

Note that the device properties for M2D are determined with the extent in which they are a result of existing presumed materials, while in D2M they include data-based modelling and/or access to databases that aim at finding a back-tuning of the materials properties that optimise the device ones. It also includes creating materials modelling workflows on demand, and materials informatics approaches (big data).

Table 1 lists specific features, along with the categorisation to M2D or D2M and the 3 prioritized personas and workflows (modelling workflows and potential MODA's).

Note: Features 1-8 are the ones proposed in the DoA as test-case properties that will be explicitly implemented, calculated, and distributed in the IM2D workflows; the others complete the list of possible user stories.

	Feature	**M2D**	**D2M**	**Persona(s) No.**	**Workflows (MODA)**
1.	Ground state atomistic structure	X		3	DFT, MODA No. 1
2.	Energy band-gap	X		3	DFT, MODA No. 2
3.	DOS	X		3	DFT, MODA No. 2
4.	Phonon DOS	X		3	DFT, MODA No. 3
5.	Defect formation energy	X	X	2, 3	DFT, MODA No. 1
6.	Defect energies	X	X	2, 3	DFT, MODA No. 1
7.	Defect charge type: acceptor or donor	X	X	2 , 3	DFT, MODA No. 1
8.	NEB – activation energy for diffusion	X	X	1,2, 3	DFT
9.	Remnant polarization		X	1, 2	
10.	Electron affinity	X		2, 3	
11.	m^* – carrier effective mass	X	X	2, 3	DFT

12.	m^*_{tunn} – carrier tunneling effective mass		X	1, 2	
13.	λ_{th} – thermal conductivity	X		2, 3	DFT
14.	ε – permittivity	X		2, 3	DFT
15.	μ_e – carrier mobility	X		2, 3	DFT
16.	WF – work function (for metals)	X	X	1, 2, 3	DFT
17.	E_c – coercive electric field		X	1 ,2	
18.	E_g vs. T – Energy gap dependence on temperature	X		2, 3	
19.	Switching time in ferroelectric device and OTS selectors		X	2, 3	
20.	I-V curves on FET, MIM/MIS cap, 2 terminal memory devices also as a function of different temperature		X	2, 3	
21.	C-V and G-V curves on FET, MIM/MIS cap, 2 terminal memory devices also as a function of different frequency		X	2, 3	
22.	FET threshold voltage		X	2, 3	
23.	Retention measurements of Fe-RAM and Phase Change Memory (PCM), also as a function of temperatures		X	2, 3	
24.	Endurance measurements of Fe-RAM and PCM, also as a function of temperatures		X	2, 3	

Table 1 – List of specific features along with categorisation to M2D or D2M, personas and workflows (modelling workflows and potential MODA's).

4.1.3 User stories

The user stories can be constructed directly from Table 1 by following these templates depending on the class:

1. For the D2M case:

   As a <pick persona>, I want to find the combination of materials and properties with <feature> to obtain <pick device behavior>.

2. For the M2D case:
   As a <pick persona>, I want to find the <pick device feature> given <pick material property>.

For each class, we considered a set of user stories customized onto the prototypical profiles of the prioritized persona, described in Sec. 4.1.1 .

Material-to-device:

- **Persona #1 (Process engineer in a company):**
  - „As an engineer for physical electronics, I want to…"
    - „ … perform simulations with Ginestra™ to model the physical properties of electronic devices such as …"
      - „ … capacitance, electric conductance, electric leakage current etc. "
    - „ ... but I need specific other physical quantities (materials properties) as input for my computations from other DFT models available through AiiDA such as …"
      - „ … bandgap, effective mass, defect distribution, defect charges, defect formation energies, etc …"
    - „ … I wish AiiDA to give me the representative defect properties by its chemical formula …"
    - „ … and do not need to understand the complexity of a DFT simulation…"
- **Persona #2 (Engineer in a company):**
  - „As an engineer in a company, I am a practical working researcher, have experience and theoretical background in the characterization of materials …"
  - „… and I do not want to worry about the technical complexity of simulations …"
  - „… but I am open to learn about new scientific aspects, concepts and models even if they are only formalized on a more general level…"
- **Profile persona #3 (DFT Researcher):**
  - „As an advanced researcher expert in DFT models, crystallography and quantum mechanics, I want to …"
  - „ … run electronic models for specific materials using AiiDA, but I want to explore its capabilities by adjusting the simulation parameters that are more advanced and fulfil my scientific interest…"

- „ ... and I want to have access to a library in Ginestra™ for the most common electronic devices (such as PCM and capacitors) with predefined, reasonable properties …“
-

Device to material:

- **Profile persona #1 and #2:**
  - „As a(n) (process) engineer in a company, I am a potential user of the D2M-workflow in Ginestra™ …”
  - „ … and I want to automatically find the most suitable material with a certain chemical formula and (defective) crystal structure…“
  - „ … which fulfils the material properties (like e.g. defect density, defect distribution, defect charges, defect formation energies, etc.) I extracted from my device-model in Ginestra™ …“
  - „ … by querying the AiiDA data-hub by the very properties of this unknown material.“
- **Profile persona #3:**
  - „As an advanced researcher of DFT models, crystallography and quantum mechanics, …“
  - „ ... I want to run simple experiments in Ginestra™ with reasonable default device properties …“
  - „ ... in order to optimize the discovery of the potential materials which are fulfilling the (defect-)properties needed for the device simulation …“
  - „ ... by controlling the complexity of the query for the AiiDA-data hub with respect to my scientific disciplinary level.“

4.1.4 Extended user stories (EPICS)

Depending on the persona profile, a potential workflow for the M2D based on the GUI can look like:

- User who is <persona… > fires up the IM2D
  - This can be done either on
    - A desktop
    - MarketPlace web platform
    - Materials Cloud/AiiDA Lab
    - Directly Ginestra™ GUI (this is a separate user story not covered in this deliverable)
  - User chooses the M2D option
  - User is presented with a number of template workflows
  - User chooses the appropriate workflow
  - User is presented with an interface to enter the parameters for each step
  - User enters the parameters
  - User submits the simulation
  - Depending on the workflow:

- Workflow that requires DFT calculations: in this case, the user is presented with an information box: calculations have started,
  - if on web user is advised to visit his/her dashboard to check on the results
  - if on desktop user is advised to send the application to the background
  - user receives a notification when the calculation is over.
- Workflow without DFT calculations
  - User sees a "Wait, doing calculation" info box.

- Once the calculation is over:
  - User can review results and relevant plots
  - User can choose whether to store in the local database or discard calculation
  - User can choose to donate the results to open databases.

4.2 EMMC Modelling DATA: MODA

This section focuses on the development of the EMMC MODA workflows for the M2D design application case. The MODA workflow diagrams provide a standard description of the modelling approach, and it is used to identify user cases, physics equations, materials relations, numerical data, and the pre and post processed elements required to fulfil the IM2D specifications (Figure 2).

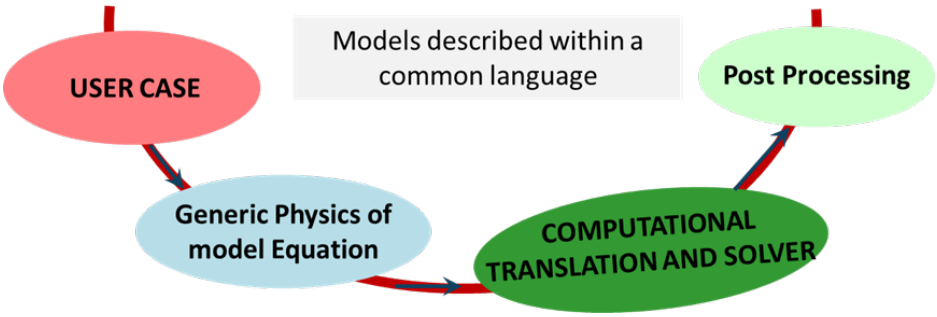


Figure 2 – MODA schema.

4.2.1 MODA for Material-to-device design

The presented MODA for Material-to-device design is generic enough and hence valid for all the user cases. The modelling structure is always the same involving an initial electronic DFT model followed by an atomistic kinetic Monte Carlo model and finally a continuous Drift-Diffusion model. The major differences among the user cases will be related to the material and material-property under investigation.

The MODA workflows will be described within the following sections that comprise the description of workflow and its rationale (4.2.1.1) followed by the workflow diagrams (4.2.1.2).

4.2.1.1 Workflow and its rationale

User case: Material-to-device design

In addition to the specification of device type and the applied voltages, the electrical characterization of synaptic devices (e.g., PCM) requires a few input parameters (such as the electronic DOS and bandgap, electronic and thermal conductivities, etc.) that are strictly dependent on the specific (i.e., not-ideal) characteristic of the material sample in that device configuration. These material sample characteristics include stoichiometry, vacancies, doping level, etc. Since such material parameters are not usually available in standard databases, specific electron and atomic model simulations are necessary for material characterization.
Thus, the modelling approach consists of 3 different model types: an electronic Density Functional Theory (DFT) model (model type 1), an atomistic kinetic Monte Carlo model (model type 2) and a continuum Drift-Diffusion model (model type 3).

- Model type 1 provides a microscopic analysis of the electron-derived ground-state properties of the materials at T=0K in terms of atomic structure, electronic density of states, defect distribution, defect formation enthalpies, and vibrational frequencies.

- Model type 2 exploits such data as input to establish the atomic structure, the defects dynamics and the phase transition properties at working temperature. The processed output of this step (e.g. conductivities and scattering rates) enters as material descriptor in model 3, where the simulation of the device is carried out.

- Model type 3 is a continuum Drift-Diffusion model that aims at evaluating the electrical performance of the material.

4.2.1.2 Workflow diagram

The MODA workflow diagram that describes the complete modelling process of the Material-to-device user case is represented in Figure 3. In this workflow, the electronic DFT model has threefold objective: determination of the defect formation enthalpy, band gap and DOS, and the vibrational properties. The electronic DFT models for the determination of the band gap and DOS and the determination of the vibrational properties are represented in Figure 4 and Figure 5 respectively, and have been described in different MODAS, MODA 2 and MODA 3. The outputs of these MODAs are used as input in the atomistic kinetic Monte Carlo model described in the overall modelling workflow in Figure 3. The electronic DFT model used to determine the defect formation enthalpy of a binary material (such as GeSe or HfO_2) is represented in Figure 2 and involves four independent steps which are represented as four different models (model 1, model 2, model 3, and model 4):

- Model 1 determines the total energy of the system under ideal conditions (with no defect);
- Model 2 determines the total energy of the defect structure;
- Model 3 determines the total energy of the pure element 1 that constitutes the material;
- Model 4 determines the total energy of the pure element 2 that constitutes the material.

The defect formation enthalpy for a defect is obtained using the output of these four electronic DFT models. For a defect D in the charge state q, the defect formation enthalpy can be calculated from the following expression:

$$\Delta H = E(D^q) - E(bulk) + \sum_i \Delta n_i \mu_i + q(E_f + E_{VBT})$$

where, $E(D^q)$ and $E(bulk)$ are the total energy of the system with and without the defect obtained from model 2 and model 1, respectively; μ_i is the chemical potential that can be calculated on the basis of the energy of each pure material (model 3 and 4 respectively), and E_{VBT} is the valence band top energy obtained from DOS of the bulk system (model 1).
Currently, this type of post-processing, single data-based model that requires input from different models is not supported by the MODA APP, therefore the four electronic DFT models have been added as independent models from both the atomistic kinetic Monte Carlo and the continuum Drift-Diffusion model, and have been edited and linked afterwards. Having the flexibility to describe post-processing in this way is part of the upcoming features portfolio.
The extended tabular description of each proposed MODA, as resulting from online MODA APP, is attached at the end of this deliverable (see the Appendix).

Figure 3 - MODA 1 workflow diagram for Material-to-device design modelling approach.

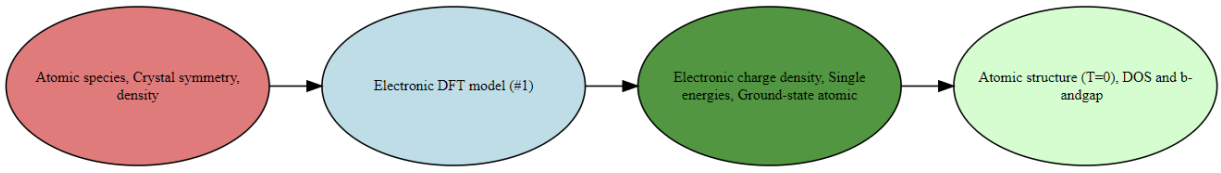


Figure 4 - MODA 2: workflow diagram for electronic DFT model for determination of bandgap and DOS.

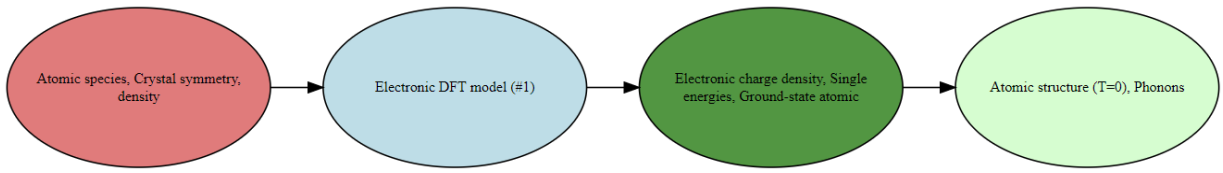


Figure 5 - MODA 3: workflow diagram for electronic DFT model for determination of the vibrational properties.

4.3 System Requirements

Based on the analysis of the user cases, the following requirements are formulated. These will be further formalized into the Unified Modelling Language (UML) diagrams on the remaining tasks in this WP.

1. The system has the ability to allow the user to define the feature(s) they are interested in:
    a. Rational: all user stories and usage scenarios are focused on the features the user is interested in.
    b. Risks: focusing on features may result in limited functionality.
    c. Mitigation: extend functionality or provide modular user interfaces.
2. The system has to support both D2M and M2D scenarios
    a. Rational: IM2D has to cater for two main scenarios. In the first, the available materials and their known properties are a limitation on the device properties. This is the traditional approach. In the second, more ambitious and innovative approach, the device properties are not limited to the available materials or their properties, but rather the designer (the user) is primarily interested in adapting the materials and their properties to the performance. The question of whether such a material exists or is feasible, is out of the scope of INTERSECT.
    b. Risks: it may be too complex to support the D2M approach, due to the need for large existing databases of relevant materials properties, and to the lack of validation.
    c. Mitigations: add functionality gradually and populate the databases using the IM2D system itself.
3. Preset, modular, integrated workflows can be tuned to specific given use cases
    a. Rationale: the MODA for the most relevant applications are fairly standardized, in the sense that each application case differs in the materials components (stoichiometry), crystalline structures, band-structure, microstructure, dopants, and so on, but the models and the chain of models are largely fixed. Hence, a set of preset workflows can be offered with some limited modularity for the user. Another advantage is that each of the workflows can be well tested and hence avoid errors by inexperienced users.
    b. Risks: Workflows are not representative of actual real user cases or insufficient.
    c. Mitigation: it develops new workflows and plug them into the system.
4. The System must support ontology-based interoperability:
    a. Rational: there is a need to exchange multiple models and methods. The results of such simulations are often large data-sets. It is important to be

able to store them into databases and enable semantic services to find the most relevant data. This is especially true for the D2M approach, where extensive use of data-based modelling and on demand high throughput simulations is needed. Moreover, integration to semantic platforms such as MarketPlace becomes much easier. Maintenance and upscaling of the tools is easier.

b. Risks: Ontology development is difficult, support for multiple models and tools, including workflows, is too cumbersome. Moreover, there may be a chance that no real immediate value for ontology use in general, and for EMMO in particular, may be obvious for applications in INTERSECT.
c. Mitigation: focus ontology on the most needed concepts in INTERSECT, apply to one case at a time, prove and demonstrate benefit.

5. Integrate all models through AiiDA and develop an interoperable interface to AiiDA by using SimPhoNy OSP-CORE (note that this is the case described in Figure 4 of the DoA and also shown below in Figure 6).
    a. Rational:
        1. AiiDA already supports many codes and plugins, and new ones can be rapidly developed. Hence, this is a major advantage.
        2. AiiDA support is syntactic in the sense that it preserves input and output, pre and post processing, and terminology and concepts of the respective tools. Adding a semantic interface to AiiDA from scratch may disrupt the functioning of multiple integrated plugins and codes.
        3. SimPhoNy-OSP core provides out of the box semantic interoperability based on an ontology and supports EMMO.
        4. Building new interfaces to all tools directly using OSP-CORE compliant wrappers is time consuming.
        5. Rendering the existing AiiDA plugins semantic is an option, but also time consuming, and would not be fully semantic anyway because AiiDA itself is not ontology based (semantic is used here as in ontology-based).
        6. Wrapping AiiDA with SimPhoNy creates a good match where the strength of each application is preserved but jointly provides a fully interoperable semantic system to the outside.
    b. Risk: the implementation of a generic AiiDA SimPhoNy wrapper may be too complex.
    c. Mitigation: focus the wrapper to the cases needed in INTERSECT.

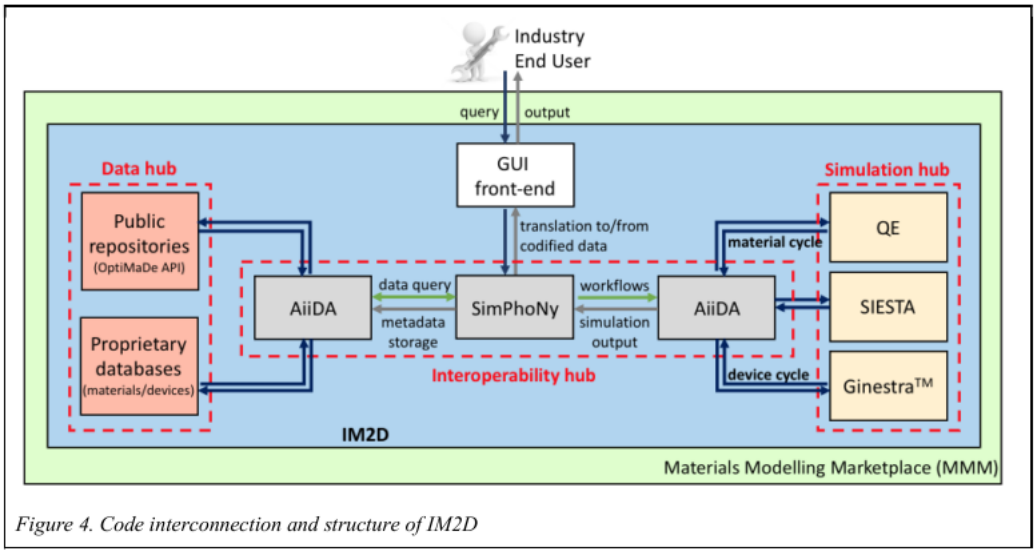


Figure 4. Code interconnection and structure of IM2D

Figure 6 - Picture from DoA.

ACRONYMS

D2M - Device-to-Material
DFT - Density Functional Theory
DoA - Description of the Action
DOS - Density of State
EMMC - European Materials Modelling Council
EMMO - European Materials Modelling Ontology
EPICS - Extended User Application Cases Stories
GUI - Graphical User Interface
iHub - interoperability Hub
IM2D - Interoperable Materials-To-Device
M2D - Material-to-Device
MODA - Materials Modeling Metadata
PCM - Phase Change Memory
QE - Quantum ESPRESSO
UML - Unified Modelling Language

APPENDIX

EXTENDED MODA DESCRIPTION

The European Materials Modelling Council

MODA Portal [Release Candidate 1.0]

USER CASE: Material-to-device design - MODA1

PROJECT (NAME/ACRONYM): Intersect

OVERVIEW OF THE SIMULATION

DESCRIPTION: Material-to-device design: optimization of the characteristics of synaptic electronic devices (such as ferroelectric-based logic, PCM memories and selectors) from the characterization, control and tuning of the materials.

PUBLICATION(S) PEERREVIEWING THE SIMULATION:

ACCESS CONDITIONS: Electronic model: Programs Quantum-Espresso (QE, www.quantum-espresso.org) and SIESTA (www.icmab.es/siesta) are open source codes. Atomistic and continuum model: Program Ginestra® is commercially distributed by MDLab.

WORKFLOW AND ITS RATIONALE: Beside the specification of device type and the applied voltages, the electrical characterization of synaptic devices (e.g. RRAM) requires a few input parameters (such as the electronic, ionic and thermal conductivities, as well as the inelastic scattering rates) that are strictly dependent on the specific (i.e. not-ideal) characteristic of the material sample in that device configuration, including stoichiometry, vacancies, doping level, etc. Since such material parameters are not usually available in standard databases, specific electron and atomic model simulations are necessary for material characterization. Thus, model 1 provides a microscopic (DFT based) analysis of electron-derived ground-state properties of materials at T=0K in terms of atomic structure, density of states, defect distribution and formation enthalpies. Model 2 exploits such data as input to establish the atomic structure, the defects dynamics and the phase transition properties at working temperature. The processed output of this step (e.g. conductivities and scattering rates) enters as material descriptor in model 3, where the simulation of the device is carried out. Model 3 is a continuum Drift-Diffusion model that aims at evaluating the electrical performance of the material.

MODELS

MODEL 1

LINKED TO MODEL(S):

COUPLED TO MODEL(S):

MODEL NAME:
Electronic DFT model (Recovered)

1. ASPECT OF THE USER CASE/SYSTEM TO BE SIMULATED

ASPECT TO BE SIMULATED: Determination of the ground-state properties of material at T=0K in terms of atomic structure, density of states, defect distribution and formation enthalpies.

MATERIAL: Semiconductor materials such as Ferroelectric HfO2, ovonic chalcogenides (GeSe, GST) with various distributions of defects.

GEOMETRY: 3D bulk crystalline and amorphous phases. Database for crystalline structures: ICSD

TIME LAPSE: N/A

MANUFACTURING PROCESS OR IN-SERVICE CONDITIONS: External temperature (T1) in the range of 300 -700K

USER CASE INPUT Atomic species, Ideal structure (without defects)

(DISPLAYED IN WORKFLOW):

PUBLICATION(S) ON THIS DATA:

2. GENERIC PHYSICS OF THE MODEL EQUATION

PHYSICS EQUATIONS

EQUATION SET 1

MAIN TYPE: Electronic Models

SUBTYPE 1: Kohn Sham equation Density Functional Theory (electronic DFT)

ENTITY: Electron

MODEL (EQUATION SET) NAME: Density Functional Theory (DFT) model

MODEL (EQUATION SET) DESCRIPTION: Kohn–Sham (KS) equation

EQUATIONS:

EQUATION 1

EQUATION PREVIEW:

$$[-\frac{1}{2}\nabla^2 + V_{eff}(r)]\psi(\mathbf{r}) = \epsilon_i\psi_i(\mathbf{r})$$

$$\rho(\mathbf{r}) = \sum |\psi_i(\mathbf{r})|^2$$

PHYSICS QUANTITIES

QUANTITY 1

NAME: Electronic charge density

SYMBOL: $\rho(\mathbf{r})$

DESCRIPTION:

QUANTITY 2

NAME: Single particle energies

SYMBOL: ϵ_i

DESCRIPTION:

QUANTITY 3

NAME: Ground-state atomic positions

SYMBOL: $R_I, I = 1, \ldots, N$

DESCRIPTION: Real space atomic position of atoms

MATERIALS RELATIONS

RELATION 1

NAME: Effective potential

DESCRIPTION:

EQUATION PREVIEW:

$$V_{eff} = V_{ext} + V_H + V_{xc}$$

PHYSICS QUANTITIES

RELATION 2

NAME: Exchange correlation potential

DESCRIPTION: Exchange correlation potential calculation based on the Generalized Gradient approximation (GGA) to exchange correlation functional (e.g. Perdew, Burke and Ernzerhof (PBE) formulation)

EQUATION PREVIEW:

$$V_{xc} = \frac{\delta E_{xc}[\rho]}{\delta\rho(\mathbf{r})}$$

PHYSICS QUANTITIES

RELATION 3

NAME: External potential

DESCRIPTION: External Coulomb potential due to atomic ions

EQUATION PREVIEW: $V_{ext} = \frac{Ze^2}{R_I - r}$

PHYSICS QUANTITIES

RELATION 4

NAME: Hartree potential

DESCRIPTION:

EQUATION PREVIEW: $V_H = e^2 \int \frac{\rho(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|} d\mathbf{r}'$

PHYSICS QUANTITIES

The simulated input is an output of another model, as defined in the workflow.

3. SOLVER AND COMPUTATIONAL TRANSLATION OF THE SPECIFICATIONS

NUMERICAL SOLVER: Iterative Self-consistent eld (scf) eigensolver for DFT problem Davidson or Conjugated gradient - electronic structure BFGS quasi-newton algorithm - optimization of atomic structure

SOFTWARE TOOL: Quantum-Espresso (QE) (QE, www.quantum-espresso.org) and SIESTA (www.icmab.es/siesta)

TIME STEP: N/A

COMPUTATIONAL REPRESENTATION

PHYSICS EQUATION: DFT problem is solved for a set of valence electrons corresponding to the atoms in the simulation cell. Kohn-Sham equation is represented in the matrix form. Eigenvectors (eigenvalues) of KS equation are the single particle wavefunctions (energies) of the matrix problem. Monkhorst-Pack mesh is used for Brillouin zone sampling and k-summation.

MATERIAL RELATIONS: Single particle KS orbitals and charge density are expanded on plane-wave basis set in QE or finite-range pseudo-atomic orbital (PAO) in SIESTA. Charge density and potential are calculated on FFT grids

MATERIAL: Nuclei are represented by points in the real space, whose charge is defined by the corresponding pseudopotential.

COMPUTATIONAL BOUNDARY CONDITIONS: Periodic boundary conditions

ADDITIONAL SOLVER PARAMETERS: Atomic structures are relaxed until forces on all atoms become lower than 0.03 eV/Ang-1. Kinetic Cut off and PAO basis set depend on specific material simulation.

4. POST PROCESSING

THE PROCESSED OUTPUT: Total energy, Valence band top

METHODOLOGIES: Defect formation enthalpy for defect D in the charge state q is obtained from expression: ΔH=E(D^q)-E(bulk)+sum(Δn_i μ_i + q(E_f + E_VBT)) where, E(D^q) and E(bulk) are the total energy of the system with and without the defect, respectively; Δni is the number of atoms exchanged between the supercell and the reservoir of energy μ_i ; q is the number of electrons exchanged between the supercell and the reservoir of energy E_f (Fermi level).

MARGIN OF ERROR: Margin of error: ~ 10%. Mostly due to the error in the material relations (e.g. exchange and correlation functionals).

MODEL 2

LINKED TO MODEL(S):

COUPLED TO MODEL(S):

MODEL NAME:
Electronic DFT model

1. ASPECT OF THE USER CASE/SYSTEM TO BE SIMULATED

ASPECT TO BE SIMULATED: Determination of the ground-state properties of material at T=0K in terms of atomic structure, density of states, defect distribution and formation enthalpies.

MATERIAL: Semiconductor materials such as Ferroelectric HfO2, ovonic chalcogenides (GeSe, GST) with various distributions of defects.

GEOMETRY: 3D bulk crystalline and amorphous phases.

TIME LAPSE: N/A

MANUFACTURING PROCESS OR IN-SERVICE CONDITIONS: External temperature (T1) in the range of 300 -700K

USER CASE INPUT (DISPLAYED IN WORKFLOW): Atomic species, Defective structure

PUBLICATION(S) ON THIS DATA:

2. GENERIC PHYSICS OF THE MODEL EQUATION

PHYSICS EQUATIONS

EQUATION SET 1

MAIN TYPE: Electronic Models

SUBTYPE 1: Kohn Sham equation Density Functional Theory (electronic DFT)

ENTITY: Electron

MODEL (EQUATION SET) NAME: Density Functional Theory (DFT) model

MODEL (EQUATION SET) DESCRIPTION: Kohn–Sham (KS) equation

EQUATIONS:

EQUATION 1

EQUATION PREVIEW:

$$[-\frac{1}{2}\nabla^2 + V_{eff}(r)]\psi(\mathbf{r}) = \epsilon_i\psi_i(\mathbf{r})$$

$$\rho(\mathbf{r}) = \sum |\psi_i(\mathbf{r})|^2$$

PHYSICS QUANTITIES

QUANTITY 1
NAME: Electronic charge density
SYMBOL: $\rho(\mathbf{r})$
DESCRIPTION:

QUANTITY 2
NAME: Single particle energies
SYMBOL: ϵ_i
DESCRIPTION:

QUANTITY 3
NAME: Ground-state atomic position
SYMBOL: $R_I, I = 1, \ldots, N$
DESCRIPTION:

MATERIALS RELATIONS

RELATION 1

NAME: Effective potential

DESCRIPTION:

EQUATION PREVIEW:

$$V_{eff} = V_{ext} + V_H + V_{xc}$$

PHYSICS QUANTITIES

RELATION 2

NAME: Exchange correlation potential

DESCRIPTION: Exchange correlation potential calculation based on the Generalized Gradient approximation (GGA) to exchange correlation functional (e.g. Perdew, Burke and Ernzerhof (PBE) formulation)

EQUATION PREVIEW: $V_{xc} = \frac{\delta E_{xc}[\rho]}{\delta \rho(\mathbf{r})}$

PHYSICS QUANTITIES

RELATION 3

NAME: External potential

DESCRIPTION: External Coulomb potential due to atomic ions

EQUATION PREVIEW: $V_{ext} = \frac{Ze^2}{R_I - r}$

PHYSICS QUANTITIES

RELATION 4

NAME: Hartree potential

DESCRIPTION:

EQUATION PREVIEW: $V_H = e^2 \int \frac{\rho(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|} d\mathbf{r}'$

PHYSICS QUANTITIES

The simulated input is an output of another model, as defined in the workflow.

3. SOLVER AND COMPUTATIONAL TRANSLATION OF THE SPECIFICATIONS

NUMERICAL SOLVER: Iterative Self-consistent eld (scf) eigensolver for DFT problem Davidson or Conjugated gradient - electronic structure BFGS quasi-newton algorithm - optimization of atomic structure

SOFTWARE TOOL: Quantum-Espresso (QE) (QE, www.quantum-espresso.org) and SIESTA (www.icmab.es/siesta)

TIME STEP: N/A

COMPUTATIONAL REPRESENTATION

PHYSICS EQUATION: DFT problem is solved for a set of valence electrons corresponding to the atoms in the simulation cell. Kohn-Sham equation is represented in the matrix form. Eigenvectors (eigenvalues) of KS equation are the single particle wavefunctions (energies) of the matrix problem. Monkhorst-Pack mesh is used for Brillouin zone sampling and k-summation.

MATERIAL RELATIONS: Single particle KS orbitals and charge density are expanded on plane-wave basis set in QE or finite-range pseudo-atomic orbital (PAO) in SIESTA. Charge density and potential are calculated on FFT grids

MATERIAL: Nuclei are represented by points in the real space, whose charge is defined by the corresponding pseudopotential.

COMPUTATIONAL BOUNDARY CONDITIONS: Periodic boundary conditions

ADDITIONAL SOLVER PARAMETERS: Atomic structures are relaxed until forces on all atoms become lower than 0.03 eV/Ang-1. Kinetic Cut off and PAO basis set depend on specific material simulation.

4. POST PROCESSING

THE PROCESSED OUTPUT: Total energy of defect structure

METHODOLOGIES: Defect formation enthalpy for defect D in the charge state q is obtained from expression: ΔH=E(D^q)-E(bulk)+sum(Δn_i μ_i + q(E_f + E_VBT)) where, E(D^q) and E(bulk) are the total energy of the system with and without the defect, respectively; Δni is the number of atoms

exchanged between the supercell and the reservoir of energy μ_i ; q is the number of electrons exchanged between the supercell and the reservoir of energy E_f (Fermi level).

MARGIN OF ERROR: Margin of error: ~ 10%. Mostly due to the error in the material relations (e.g. exchange and correlation functionals).

MODEL 3

LINKED TO MODEL(S):

COUPLED TO MODEL(S):

MODEL NAME:
Electronic DFT model

1. ASPECT OF THE USER CASE/SYSTEM TO BE SIMULATED

ASPECT TO BE SIMULATED: Determination of the ground-state properties of material at T=0K in terms of atomic structure, density of states, defect distribution and formation enthalpies.

MATERIAL: Semiconductor materials such as Ferroelectric HfO2, ovonic chalcogenides (GeSe, GST) with various distributions of defects.

GEOMETRY: 3D bulk crystalline and amorphous phases.

TIME LAPSE: N/A

MANUFACTURING PROCESS OR IN-SERVICE CONDITIONS: External temperature (T1) in the range of 300 -700K

USER CASE INPUT (DISPLAYED IN WORKFLOW): Atomic species, Pure element 1 structure

PUBLICATION(S) ON THIS DATA:

2. GENERIC PHYSICS OF THE MODEL EQUATION

PHYSICS EQUATIONS

EQUATION SET 1

MAIN TYPE: Electronic Models

SUBTYPE 1: Kohn Sham equation Density Functional Theory (electronic DFT)

ENTITY: Electron

MODEL (EQUATION SET) NAME: Density Functional Theory (DFT) model

MODEL (EQUATION SET) DESCRIPTION: Kohn–Sham (KS) equation

EQUATIONS:

EQUATION 1

EQUATION PREVIEW:

$$[-\frac{1}{2}\nabla^2 + V_{eff}(r)]\psi(\mathbf{r}) = \epsilon_i\psi_i(\mathbf{r})$$

$$\rho(\mathbf{r}) = \sum |\psi_i(\mathbf{r})|^2$$

PHYSICS QUANTITIES

QUANTITY 1
NAME: Electronic charge density
SYMBOL: $\rho(\mathbf{r})$
DESCRIPTION:

QUANTITY 2
NAME: Single particle energies
SYMBOL: ϵ_i
DESCRIPTION:

QUANTITY 3
NAME: Ground-state atomic

SYMBOL: $R_I, I = 1, \ldots, N$

DESCRIPTION: Real space atomic position of atoms

MATERIALS RELATIONS

RELATION 1

NAME: Effective potential

DESCRIPTION:

EQUATION PREVIEW: $V_{eff} = V_{ext} + V_H + V_{xc}$

PHYSICS QUANTITIES

RELATION 2

NAME: Exchange correlation potential

DESCRIPTION: Exchange correlation potential calculation based on the Generalized Gradient approximation (GGA) to exchange correlation functional (e.g. Perdew, Burke and Ernzerhof (PBE) formulation)

EQUATION PREVIEW: $V_{xc} = \frac{\delta E_{xc}[\rho]}{\delta \rho(\mathbf{r})}$

PHYSICS QUANTITIES

RELATION 3

NAME: External potential

DESCRIPTION: External Coulomb potential due to atomic ions

EQUATION PREVIEW: $V_{ext} = \frac{Ze^2}{R_I - r}$

PHYSICS QUANTITIES

RELATION 4

NAME: Hartree potential

DESCRIPTION:

EQUATION PREVIEW: $V_H = e^2 \int \frac{\rho(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} d\mathbf{r}'$

PHYSICS QUANTITIES

The simulated input is an output of another model, as defined in the workflow.

3. SOLVER AND COMPUTATIONAL TRANSLATION OF THE SPECIFICATIONS

NUMERICAL SOLVER: Iterative Self-consistent eld (scf) eigensolver for DFT problem Davidson or Conjugated gradient - electronic structure BFGS quasi-newton algorithm - optimization of atomic structure

SOFTWARE TOOL: Quantum-Espresso (QE) (QE, www.quantum-espresso.org) and SIESTA (www.icmab.es/siesta)

TIME STEP: N/A

COMPUTATIONAL REPRESENTATION

PHYSICS EQUATION: DFT problem is solved for a set of valence electrons corresponding to the atoms in the simulation cell. Kohn-Sham equation is represented in the matrix form. Eigenvectors (eigenvalues) of KS equation are the single particle wavefunctions (energies) of the matrix problem. Monkhorst-Pack mesh is used for Brillouin zone sampling and k-summation.

MATERIAL RELATIONS: Single particle KS orbitals and charge density are expanded on plane-wave basis set in QE or finite-range pseudo-atomic orbital (PAO) in SIESTA. Charge density and potential are calculated on FFT grids.

MATERIAL: Nuclei are represented by points in the real space, whose charge is defined by the corresponding pseudopotential.

COMPUTATIONAL BOUNDARY CONDITIONS: Periodic boundary conditions

ADDITIONAL SOLVER PARAMETERS: Atomic structures are relaxed until forces on all atoms become lower than 0.03 eV/Ang-1. Kinetic Cut off and PAO basis set depend on specific material simulation.

4. POST PROCESSING

THE PROCESSED OUTPUT: Total energy of pure element 1

METHODOLOGIES: Defect formation enthalpy for defect D in the charge state q is obtained from expression: ΔH=E(D^q)-E(bulk)+sum(Δn_i μ_i + q(E_f + E_VBT)) where, E(D^q) and E(bulk) are the total energy of the system with and without the defect, respectively; Δni is the number of atoms exchanged between the supercell and the reservoir of energy μ_i ; q is the number of electrons exchanged between the supercell and the reservoir of energy E_f (Fermi level).

MARGIN OF ERROR: Margin of error: ~ 10%. Mostly due to the error in the material relations (e.g. exchange and correlation functionals).

MODEL 4

LINKED TO MODEL(S):

COUPLED TO MODEL(S):

MODEL NAME:
Electronic DFT model

1. ASPECT OF THE USER CASE/SYSTEM TO BE SIMULATED

ASPECT TO BE SIMULATED: Determination of the ground-state properties of material at T=0K in terms of atomic structure, density of states, defect distribution and formation enthalpies.

MATERIAL: Semiconductor materials such as Ferroelectric HfO2, ovonic chalcogenides (GeSe, GST) with various distributions of defects.

GEOMETRY: 3D bulk crystalline and amorphous phases. Database for crystalline structures: ICSD

TIME LAPSE: N/A

MANUFACTURING PROCESS OR IN-SERVICE CONDITIONS: External temperature (T1) in the range of 300 -700K

USER CASE INPUT (DISPLAYED IN WORKFLOW): Atomic species, Pure element 2 structure

PUBLICATION(S) ON THIS DATA:

2. GENERIC PHYSICS OF THE MODEL EQUATION

PHYSICS EQUATIONS

EQUATION SET 1

MAIN TYPE: Electronic Models

SUBTYPE 1: Kohn Sham equation Density Functional Theory (electronic DFT)

ENTITY: Electron

MODEL (EQUATION SET) NAME: Density Functional Theory (DFT) model

MODEL (EQUATION SET) DESCRIPTION: Kohn–Sham (KS) equation

EQUATIONS:

EQUATION 1

EQUATION PREVIEW:

$$[-\frac{1}{2}\nabla^2 + V_{eff}(r)]\psi(\mathbf{r}) = \epsilon_i\psi_i(\mathbf{r})$$

$$\rho(\mathbf{r}) = \sum |\psi_i(\mathbf{r})|^2$$

PHYSICS QUANTITIES

QUANTITY 1
NAME: Electronic charge density
SYMBOL: $\rho(\mathbf{r})$
DESCRIPTION:

QUANTITY 2
NAME: Single particle energies
SYMBOL: ϵ_i
DESCRIPTION:

QUANTITY 3
NAME: Ground-state atomic
SYMBOL: $R_I, I = 1, \ldots, N$
DESCRIPTION:

MATERIALS RELATIONS

RELATION 1
NAME: Effective potential
DESCRIPTION:
EQUATION PREVIEW: $V_{eff} = V_{ext} + V_H + V_{xc}$
PHYSICS QUANTITIES

RELATION 2
NAME: Exchange correlation potential
DESCRIPTION: Exchange correlation potential calculation based on the Generalized Gradient approximation (GGA) to exchange correlation functional (e.g. Perdew, Burke and Ernzerhof (PBE) formulation)
EQUATION PREVIEW: $V_{xc} = \frac{\delta E_{xc}[\rho]}{\delta \rho(\mathbf{r})}$
PHYSICS QUANTITIES

RELATION 3
NAME: External potential
DESCRIPTION: External Coulomb potential due to atomic ions
EQUATION PREVIEW: $V_{ext} = \frac{Ze^2}{R_I - r}$
PHYSICS QUANTITIES

RELATION 4
NAME: Hartree potential
DESCRIPTION:
EQUATION PREVIEW: $V_H = e^2 \int \frac{\rho(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} d\mathbf{r}'$
PHYSICS QUANTITIES

The simulated input is an output of another model, as defined in the workflow.

3. SOLVER AND COMPUTATIONAL TRANSLATION OF THE SPECIFICATIONS

NUMERICAL SOLVER: Iterative Self-consistent eld (scf) eigensolver for DFT problem Davidson or Conjugated gradient - electronic structure BFGS quasi-newton algorithm - optimization of atomic structure

SOFTWARE TOOL: Quantum-Espresso (QE) (QE, www.quantum-espresso.org) and SIESTA (www.icmab.es/siesta)

TIME STEP: N/A

COMPUTATIONAL REPRESENTATION

PHYSICS EQUATION: DFT problem is solved for a set of valence electrons corresponding to the atoms in the simulation cell. Kohn-Sham equation is represented in the matrix form. Eigenvectors (eigenvalues) of KS equation are the single particle wavefunctions (energies) of the matrix problem. Monkhorst-Pack mesh is used for Brillouin zone sampling and k-summation.

MATERIAL RELATIONS: Single particle KS orbitals and charge density are expanded on plane-wave basis set in QE or finite-range pseudo-atomic orbital (PAO) in SIESTA. Charge density and potential are calculated on FFT grids.

MATERIAL: Nuclei are represented by points in the real space, whose charge is defined by the corresponding pseudopotential.

COMPUTATIONAL BOUNDARY CONDITIONS: Periodic boundary conditions

ADDITIONAL SOLVER PARAMETERS: Atomic structures are relaxed until forces on all atoms become lower than 0.03 eV/Ang-1. Kinetic Cut off and PAO basis set depend on specific material simulation.

4. POST PROCESSING

THE PROCESSED OUTPUT: Total energy of pure element 2

METHODOLOGIES: Defect formation enthalpy for defect D in the charge state q is obtained from expression: ΔH=E(D^q)-E(bulk)+sum(Δn_i μ_i + q(E_f + E_VBT)) where, E(D^q) and E(bulk) are the total energy of the system with and without the defect, respectively; Δni is the number of atoms exchanged between the supercell and the reservoir of energy μ_i ; q is the number of electrons exchanged between the supercell and the reservoir of energy E_f (Fermi level).

MARGIN OF ERROR: Margin of error: ~ 10%. Mostly due to the error in the material relations (e.g. exchange and correlation functionals).

MODEL 5

LINKED TO MODEL(S): 6

COUPLED TO MODEL(S):

MODEL NAME:
Atomistic kinetic Monte Carlo model

1. ASPECT OF THE USER CASE/SYSTEM TO BE SIMULATED

ASPECT TO BE SIMULATED: Determination of the atomic configuration of the material at working temperature (T1) including the defect dynamics (e.g. generation and recombination)

MATERIAL: Ferroelectric HfO2 and ovonic chalcogenides in the device configuration,including metallic leads (e.g. TiN)

GEOMETRY: Planar capacitors, cylindrical capacitors, MOSFET transistors, FINFET transistors

TIME LAPSE: In the order of seconds

MANUFACTURING PROCESS OR IN-SERVICE CONDITIONS: External temperature (T1) in the range of 100 -700K, Voltage in the range of -5V to +5V , Frequencies in the range of 1Hz to 1GHz

USER CASE INPUT (DISPLAYED IN WORKFLOW): External temperature, Device structure and properties (DOS and bandgap (MODA 2), Vibrational properties (MODA 3)), Voltage, Frequencies

PUBLICATION(S) ON THIS DATA:

2. GENERIC PHYSICS OF THE MODEL EQUATION

PHYSICS EQUATIONS

EQUATION SET 1

MAIN TYPE: Atomistic models

SUBTYPE 1: Statistical Mechanics atomistic models

ENTITY: Atom

MODEL (EQUATION SET) NAME: kinetic Monte Carlo

MODEL (EQUATION SET) DESCRIPTION:

EQUATIONS:

EQUATION 1

EQUATION PREVIEW: $R_{tot} = \sum_{i=1}^{N_{bonds}} R_{G,i} + \sum_{i=1}^{N_D} \sum_{j=1}^{N_{DIR}} R_{D,i,j} + \sum_{i=1}^{N_D} \sum_{j=1}^{N_D} R_{R,i,j}$

PHYSICS QUANTITIES

QUANTITY 1
- **NAME:** Bond breakage rate
- **SYMBOL:** $R_{G,i}$
- **DESCRIPTION:** Rate of Bond breakage of the i-th bond

QUANTITY 2
- **NAME:** Diffusion rate
- **SYMBOL:** $R_{D,i,j}$
- **DESCRIPTION:** Diffusion rate of the i-th defect along the j-th direction

QUANTITY 3
- **NAME:** Recombination rate
- **SYMBOL:** $R_{R,i,j}$
- **DESCRIPTION:** Recombination rate between the i-th and the j-th defect

MATERIALS RELATIONS

RELATION 1

NAME: Effective energy description model

DESCRIPTION: The constant rates of all the mechanisms involved are computed through a thermally activated model

EQUATION PREVIEW: $R_{TST} = f_0 exp(-\frac{E_{A,0}-bE}{k_B T})$

PHYSICS QUANTITIES

QUANTITY 1
- **NAME:** Reaction rate constant
- **SYMBOL:** R_{TST}
- **DESCRIPTION:**

QUANTITY 2
- **NAME:** Frequency factor
- **SYMBOL:** f_0
- **DESCRIPTION:**

QUANTITY 3
- **NAME:** Boltzmann constant
- **SYMBOL:** k_B
- **DESCRIPTION:**

QUANTITY 4
- **NAME:** Activation energy
- **SYMBOL:** $E_{A,0}$
- **DESCRIPTION:** Note: for the bond breakage mechanism it corresponds is the defect formation energy from ab-initio calculations

The simulated input is an output of another model, as defined in the workflow.

3. SOLVER AND COMPUTATIONAL TRANSLATION OF THE SPECIFICATIONS

NUMERICAL SOLVER: Kinetic Monte Carlo (kMC)

SOFTWARE TOOL: Ginestra® (http://www.mdlab-software.it)

TIME STEP: N/A

COMPUTATIONAL REPRESENTATION

PHYSICS EQUATION: The total rate (PE1) corresponds to a scalar and is computed for every time. Is used to determine the "tentative reaction time" or time advancement

MATERIAL RELATIONS: Matrix with updated state of the device (e.g., species, locations etc..) used to calculate the events rates.

MATERIAL: Fixed grid of the cells size equal to default step of 3 Angstroms

COMPUTATIONAL BOUNDARY CONDITIONS: Periodic boundary conditions

ADDITIONAL SOLVER PARAMETERS:

4. POST PROCESSING

THE PROCESSED OUTPUT: Electrical conductivity, Thermal conductivity, Events rates

METHODOLOGIES: The spatial distribution of the atomic species allows to deduce the phase of the material, from which the above properties can be extracted.

MARGIN OF ERROR:

MODEL 6

LINKED TO MODEL(S):

COUPLED TO MODEL(S):

MODEL NAME:
Continuum Drift-Diffusion model

1. ASPECT OF THE USER CASE/SYSTEM TO BE SIMULATED

ASPECT TO BE SIMULATED: Determination of the full electrical response of the device (e.g. I-V, C-V, G-V) and its fundamental characteristics in terms of bias-temperature instability, electrical stress, leakage current, breakdown statistics.

MATERIAL: Ferroelectric HfO2 and ovonic chalcogenides in the device configuration (e.g. RRAM, PCM).

GEOMETRY: Planar capacitors, cylindrical capacitors, MOSFET transistors, FINFET transistors

TIME LAPSE: Both static and transient simulations are supported.

MANUFACTURING PROCESS OR IN-SERVICE CONDITIONS: Device type (e.g. RRAM, PCM), Applied external voltage (1-5V), External temperature (T1) in the range of 100 -700K, Frequencies in the range of 1Hz to 1GHz

USER CASE INPUT (DISPLAYED IN WORKFLOW): Device structure and properties, External Temperature, Voltage, Frequencies

PUBLICATION(S) ON THIS DATA:

2. GENERIC PHYSICS OF THE MODEL EQUATION

PHYSICS EQUATIONS

EQUATION SET 1

MAIN TYPE: Continuum modelling of materials

SUBTYPE 1: Fluid Mechanics

ENTITY: Continuum Volume

MODEL (EQUATION SET) NAME:

MODEL (EQUATION SET) DESCRIPTION: Tightly coupled set of PE: -Drift-Diffusion equation -Poisson equation (electrostatic potential) -Landau-Ginzburg Dynamic equation -Continuity

EQUATIONS:

EQUATION 1

EQUATION PREVIEW: $\nabla(\epsilon_0\bar{E} + \bar{P}(\bar{E})) = -\rho$

PHYSICS QUANTITIES

QUANTITY 1
NAME: Polarization vector
SYMBOL: $\bar{P}(\bar{E})$
DESCRIPTION:

EQUATION 2

EQUATION PREVIEW: $\rho_v . \frac{d\bar{P}}{dt} + \nabla_p u = 0$

PHYSICS QUANTITIES

QUANTITY 1
NAME: Polarization
SYMBOL: $\bar{P}$
DESCRIPTION:

EQUATION 3

EQUATION PREVIEW: $-\nabla(k_{TST}\nabla T) = p$

PHYSICS QUANTITIES

QUANTITY 1
NAME: Temperature
SYMBOL: T
DESCRIPTION:

EQUATION 4

EQUATION PREVIEW: $\frac{dn}{dt} = \frac{\nabla \bar{J}_n}{q} + R_n$

PHYSICS QUANTITIES

QUANTITY 1
NAME: Electron density
SYMBOL: n
DESCRIPTION:

EQUATION 5

EQUATION PREVIEW: $\frac{dp}{dt} = \frac{\nabla \bar{J}_p}{q} + R_p$

PHYSICS QUANTITIES

QUANTITY 1
NAME: Hole density
SYMBOL: p
DESCRIPTION:

EQUATION 6

EQUATION PREVIEW: $\frac{dF_{T,i}}{dt} = R_{in,T,i} - R_{out,T,i}$

PHYSICS QUANTITIES

QUANTITY 1
NAME: Trap occupancy
SYMBOL: $dF_{T,i}$
DESCRIPTION:

EQUATION 7

EQUATION PREVIEW: $\bar{J}_n = q\mu_n n\bar{E} + qD_n \nabla n$

PHYSICS QUANTITIES

QUANTITY 1

NAME: Electron drift diffusion current

SYMBOL: $\bar{J}_n$

DESCRIPTION:

EQUATION 8

EQUATION PREVIEW: $\bar{J}_p = q\mu_p p\bar{E} + qD_p \nabla p$

PHYSICS QUANTITIES

QUANTITY 1

NAME: Hole drift diffusion current

SYMBOL: $\bar{J}_p$

DESCRIPTION:

MATERIALS RELATIONS

RELATION 1

NAME: Gibb's free energy

DESCRIPTION:

EQUATION PREVIEW: $\mu = \alpha P^2 + \beta P^4 + \gamma P^6 + g(\nabla P)^6 - \bar{E}\bar{P} - \frac{\epsilon_0 \epsilon_b}{2} E^2$

PHYSICS QUANTITIES

QUANTITY 1

NAME: Ferroelectricity anisotropy constants

SYMBOL: α, β, γ

DESCRIPTION:

QUANTITY 2

NAME: Wall coupling constant

SYMBOL: g

DESCRIPTION: Domain wall coupling constant

RELATION 2

NAME: Electron/hole mob. electric field depend

DESCRIPTION:

EQUATION PREVIEW: $\mu = \frac{\mu_0}{1+\frac{\mu_0 E}{v_{sat}}}$

PHYSICS QUANTITIES

QUANTITY 1

NAME: Zero-field mobility

SYMBOL: μ_0

DESCRIPTION:

QUANTITY 2

NAME: Saturation velocity

SYMBOL: v_{sat}

DESCRIPTION:

RELATION 3

NAME: WKB Tunneling probability

DESCRIPTION: used for computing tunneling current and Trap Assisted capture and emission rates Rin,T,i and Rout,T,i

EQUATION PREVIEW:

$$P_T(r_1, r_2) = exp(-\frac{4\pi}{h} \int_{r_1}^{r_2} \sqrt{2.m.\ E_B(\bar{r})} dr)$$

PHYSICS QUANTITIES

QUANTITY 1
NAME: Plank constant
SYMBOL: h
DESCRIPTION:

QUANTITY 2
NAME: Tunneling effective mass
SYMBOL: m
DESCRIPTION:

QUANTITY 3
NAME: Barrier height
SYMBOL: $E_B(\bar{r})$
DESCRIPTION:

RELATION 4

NAME: Multiphonon transition probability
DESCRIPTION: used for computing Rin,T,i and Rout,T,i
EQUATION PREVIEW: $L(m)=(\frac{f_B +1}{f_B}^\frac{m}{2} e^{-S(2f_B+1)} I_m(2S

PHYSICS QUANTITIES

QUANTITY 1
NAME: Bose function
SYMBOL: f_B
DESCRIPTION:

QUANTITY 2
NAME: Huang-Rhys factor
SYMBOL: S
DESCRIPTION:

The simulated input is an output of another model, as defined in the workflow.

3. SOLVER AND COMPUTATIONAL TRANSLATION OF THE SPECIFICATIONS

NUMERICAL SOLVER: Finite Volume Method (FVM)

SOFTWARE TOOL: Ginestra® (http://www.mdlab-software.it)

TIME STEP: In case of a transient simulation an adaptive time step procedure is implemented.

COMPUTATIONAL REPRESENTATION

PHYSICS EQUATION: The set of tightly coupled equations are represented in the matrix form and are solved simultaneously. The equations are discretized using the finite volume method and integrated in time.

MATERIAL RELATIONS: The field variables representing the material relations are solved for each volume cell (FVM).

MATERIAL: The material is represented as a set of volume cells or elements that contain the information about the material behavior. Knowing the material behavior for each volume cell / element will enable the determination of the whole material behavior.

COMPUTATIONAL BOUNDARY CONDITIONS: Dirichlet/ Neumann boundary conditions

ADDITIONAL SOLVER PARAMETERS: N/A

4. POST PROCESSING

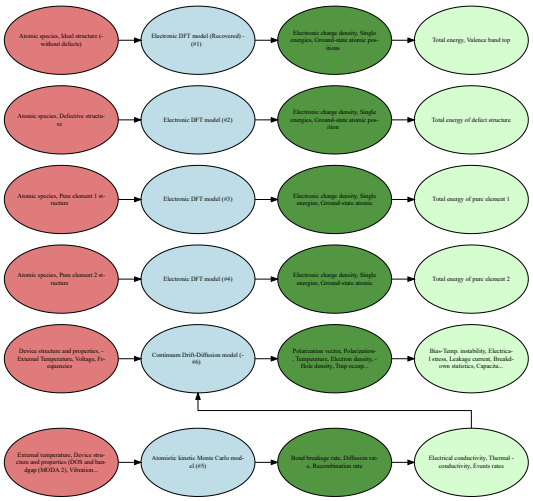
THE PROCESSED OUTPUT: Bias-Temp. instability, Electrical stress, Leakage current, Breakdown statistics, Capacitance, Conductance

METHODOLOGIES: The leakage current is computed by summing all the carrier ow rates from/to an electrode (i.e. drift diffusion, Direct and Fowler-Nordheim tunnelling, trap assisted tunnelling). The threshold voltage shift is computed through the charge sheet approximation. The time-to breakdown is computed by simulating a electrical/thermal stress and detecting the time where a certain current compliance is overtaken.

MARGIN OF ERROR: The accuracy is high if grid is refined enough and the charge transport and the device is far from the ballistic transport regime.

MODA WORKFLOW PLOT

Note: long text may not be displayed in full



The European Materials Modelling Council

MODA Portal [Release Candidate 1.0]

USER CASE: Material-to-device design - MODA 2

PROJECT (NAME/ACRONYM): Intersect

OVERVIEW OF THE SIMULATION

DESCRIPTION: Material-to-device design: optimization of the characteristics of synaptic electronic devices (such as ferroelectric-based logic, PCM memories and selectors) from the characterization, control and tuning of the materials.

PUBLICATION(S) PEERREVIEWING THE SIMULATION:

ACCESS CONDITIONS: Electronic model: Programs Quantum-Espresso (QE, www.quantum-espresso.org) and SIESTA (www.icmab.es/siesta) are open source codes. Atomistic and continuum model: Program Ginestra® is commercially distributed by MDLab.

WORKFLOW AND ITS RATIONALE: Beside the specification of device type and the applied voltages, the electrical characterization of synaptic devices (e.g. RRAM) requires a few input parameters (such as the electronic, ionic and thermal conductivities, as well as the inelastic scattering rates) that are strictly dependent on the specific (i.e. not-ideal) characteristic of the material sample in that device configuration, including stoichiometry, vacancies, doping level, etc. Since such material parameters are not usually available in standard databases, specific electron and atomic model simulations are necessary for material characterization. Thus, model 1 provides a microscopic (DFT based) analysis of electron-derived ground-state properties of materials at T=0K in terms of atomic structure, density of states, defect distribution and formation enthalpies. Model 2 exploits such data as input to establish the atomic structure, the defects dynamics and the phase transition properties at working temperature. The processed output of this step (e.g. conductivities and scattering rates) enters as material descriptor in model 3, where the simulation of the device is carried out. Model 3 is a continuum Drift-Diffusion model that aims at evaluating the electrical performance of the material.

MODELS

MODEL 1

LINKED TO MODEL(S):

COUPLED TO MODEL(S):

MODEL NAME:
Electronic DFT model (Recovered)

1. ASPECT OF THE USER CASE/SYSTEM TO BE SIMULATED

ASPECT TO BE SIMULATED: Determination of the ground-state properties of material at T=0K in terms of atomic structure, density of states, defect distribution and formation enthalpies.

MATERIAL: Semiconductor materials such as Ferroelectric HfO2, ovonic chalcogenides (GeSe, GST) with various distributions of defects.

GEOMETRY: 3D bulk crystalline and amorphous phases. Database for crystalline structures: ICSD

TIME LAPSE: N/A

MANUFACTURING PROCESS OR IN-SERVICE CONDITIONS: External temperature (T1) in the range of 300 -700K

USER CASE INPUT Atomic species, Crystal symmetry, Defect density

(DISPLAYED IN WORKFLOW):

PUBLICATION(S) ON THIS DATA:

2. GENERIC PHYSICS OF THE MODEL EQUATION

PHYSICS EQUATIONS

EQUATION SET 1

MAIN TYPE: Electronic Models

SUBTYPE 1: Kohn Sham equation Density Functional Theory (electronic DFT)

ENTITY: Electron

MODEL (EQUATION SET) NAME: Density Functional Theory (DFT) model

MODEL (EQUATION SET) DESCRIPTION: Kohn–Sham (KS) equation

EQUATIONS:

EQUATION 1

EQUATION PREVIEW:

$$[-\frac{1}{2}\nabla^2 + V_{eff}(r)]\psi(\mathbf{r}) = \epsilon_i\psi_i(\mathbf{r})$$

$$\rho(\mathbf{r}) = \sum |\psi_i(\mathbf{r})|^2$$

PHYSICS QUANTITIES

QUANTITY 1

NAME: Electronic charge density

SYMBOL: $\rho(\mathbf{r})$

DESCRIPTION:

QUANTITY 2

NAME: Single particle energies

SYMBOL: ϵ_i

DESCRIPTION:

QUANTITY 3

NAME: Ground-state atomic

SYMBOL: $R_I, I = 1, \ldots, N$

DESCRIPTION: Real space atomic position of atoms

MATERIALS RELATIONS

RELATION 1

NAME: Effective potential

DESCRIPTION:

EQUATION PREVIEW:

$$V_{eff} = V_{ext} + V_H + V_{xc}$$

PHYSICS QUANTITIES

RELATION 2

NAME: Exchange correlation potential

DESCRIPTION: Exchange correlation potential calculation based on the Generalized Gradient approximation (GGA) to exchange correlation functional (e.g. Perdew, Burke and Ernzerhof (PBE) formulation)

EQUATION PREVIEW:

$$V_{xc} = \frac{\delta E_{xc}[\rho]}{\delta\rho(\mathbf{r})}$$

PHYSICS QUANTITIES

RELATION 3

NAME: External potential

DESCRIPTION: External Coulomb potential due to atomic ions

EQUATION PREVIEW: $V_{ext} = \frac{Ze^2}{R_I - r}$

PHYSICS QUANTITIES

RELATION 4

NAME: Hartree potential

DESCRIPTION:

EQUATION PREVIEW: $V_H = e^2 \int \frac{\rho(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|} d\mathbf{r}'$

PHYSICS QUANTITIES

The simulated input is an output of another model, as defined in the workflow.

3. SOLVER AND COMPUTATIONAL TRANSLATION OF THE SPECIFICATIONS

NUMERICAL SOLVER: Iterative Self-consistent eld (scf) eigensolver for DFT problem Davidson or Conjugated gradient - electronic structure BFGS quasi-newton algorithm - optimization of atomic structure

SOFTWARE TOOL: Quantum-Espresso (QE) (QE, www.quantum-espresso.org) and SIESTA (www.icmab.es/siesta)

TIME STEP: N/A

COMPUTATIONAL REPRESENTATION

PHYSICS EQUATION: DFT problem is solved for a set of valence electrons corresponding to the atoms in the simulation cell. Kohn-Sham equation is represented in the matrix form. Eigenvectors (eigenvalues) of KS equation are the single particle wavefunctions (energies) of the matrix problem. Monkhorst-Pack mesh is used for Brillouin zone sampling and k-summation.

MATERIAL RELATIONS: Single particle KS orbitals and charge density are expanded on plane-wave basis set in QE or finite-range pseudo-atomic orbital (PAO) in SIESTA. Charge density and potential are calculated on FFT grids.

MATERIAL: Nuclei are represented by points in the real space, whose charge is defined by the corresponding pseudopotential.

COMPUTATIONAL BOUNDARY CONDITIONS: Periodic boundary conditions

ADDITIONAL SOLVER PARAMETERS: Atomic structures are relaxed until forces on all atoms become lower than 0.03 eV/Ang-1. Kinetic Cut off and PAO basis set depend on specific material simulation.

4. POST PROCESSING

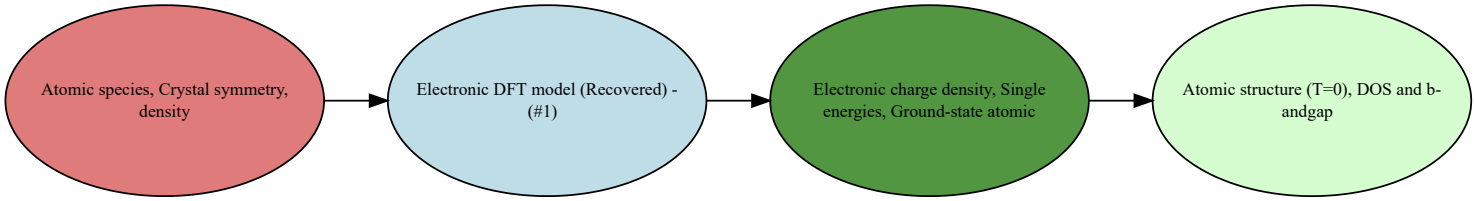
THE PROCESSED OUTPUT: Atomic structure (T=0), DOS and bandgap

METHODOLOGIES: Density of states and bandgap extracted from interpolated charge density calculated with non-self-consistent (nscf) cycle on arbitrary dense k-mesh from DFT scf density Effective masses extracted from parabolic fit from bandstruture, around valence band maxima and conduction band minima.

MARGIN OF ERROR: Margin of error: ~ 10%. Mostly due to the error in the material relations (e.g. exchange and correlation functionals).

MODA WORKFLOW PLOT

Note: long text may not be displayed in full


Atomic species, Crystal symmetry, density
Electronic DFT model (Recovered) - (#1)
Electronic charge density, Single energies, Ground-state atomic
Atomic structure (T=0), DOS and b-andgap

The European Materials Modelling Council

MODA Portal [Release Candidate 1.0]

USER CASE: Material-to-device design - MODA 3

PROJECT (NAME/ACRONYM): Intersect

OVERVIEW OF THE SIMULATION

DESCRIPTION: Material-to-device design: optimization of the characteristics of synaptic electronic devices (such as ferroelectric-based logic, PCM memories and selectors) from the characterization, control and tuning of the materials.

PUBLICATION(S) PEERREVIEWING THE SIMULATION:

ACCESS CONDITIONS: Electronic model: Programs Quantum-Espresso (QE, www.quantum-espresso.org) and SIESTA (www.icmab.es/siesta) are open source codes. Atomistic and continuum model: Program Ginestra® is commercially distributed by MDLab.

WORKFLOW AND ITS RATIONALE: Beside the specification of device type and the applied voltages, the electrical characterization of synaptic devices (e.g. RRAM) requires a few input parameters (such as the electronic, ionic and thermal conductivities, as well as the inelastic scattering rates) that are strictly dependent on the specific (i.e. not-ideal) characteristic of the material sample in that device configuration, including stoichiometry, vacancies, doping level, etc. Since such material parameters are not usually available in standard databases, specific electron and atomic model simulations are necessary for material characterization. Thus, model 1 provides a microscopic (DFT based) analysis of electron-derived ground-state properties of materials at T=0K in terms of atomic structure, density of states, defect distribution and formation enthalpies. Model 2 exploits such data as input to establish the atomic structure, the defects dynamics and the phase transition properties at working temperature. The processed output of this step (e.g. conductivities and scattering rates) enters as material descriptor in model 3, where the simulation of the device is carried out. Model 3 is a continuum Drift-Diffusion model that aims at evaluating the electrical performance of the material.

MODELS

MODEL 1

LINKED TO MODEL(S):

COUPLED TO MODEL(S):

MODEL NAME:
Electronic DFT model (Recovered)

1. ASPECT OF THE USER CASE/SYSTEM TO BE SIMULATED

ASPECT TO BE SIMULATED: Determination of the ground-state properties of material at T=0K in terms of atomic structure, density of states, defect distribution and formation enthalpies.

MATERIAL: Semiconductor materials such as Ferroelectric HfO2, ovonic chalcogenides (GeSe, GST) with various distributions of defects.

GEOMETRY: 3D bulk crystalline and amorphous phases. Database for crystalline structures: ICSD

TIME LAPSE: N/A

MANUFACTURING PROCESS OR IN-SERVICE CONDITIONS: External temperature (T1) in the range of 300 -700K

USER CASE INPUT Atomic species, Crystal symmetry, Defect density

(DISPLAYED IN WORKFLOW):

PUBLICATION(S) ON THIS DATA:

2. GENERIC PHYSICS OF THE MODEL EQUATION

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EQUATIONS:

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DESCRIPTION:

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SYMBOL: ϵ_i

DESCRIPTION:

QUANTITY 3

NAME: Ground-state atomic

SYMBOL: $R_I, I = 1, \ldots, N$

DESCRIPTION: Real space atomic position of atoms

MATERIALS RELATIONS

RELATION 1

NAME: Effective potential

DESCRIPTION:

EQUATION PREVIEW:

$$V_{eff} = V_{ext} + V_H + V_{xc}$$

PHYSICS QUANTITIES

RELATION 2

NAME: Exchange correlation potential

DESCRIPTION: Exchange correlation potential calculation based on the Generalized Gradient approximation (GGA) to exchange correlation functional (e.g. Perdew, Burke and Ernzerhof (PBE) formulation)

EQUATION PREVIEW:

$$V_{xc} = \frac{\delta E_{xc}[\rho]}{\delta\rho(\mathbf{r})}$$

PHYSICS QUANTITIES

RELATION 3

NAME: External potential

DESCRIPTION: External Coulomb potential due to atomic ions

EQUATION PREVIEW: $V_{ext} = \frac{Ze^2}{R_I - r}$

PHYSICS QUANTITIES

RELATION 4

NAME: Hartree potential

DESCRIPTION:

EQUATION PREVIEW: $V_H = e^2 \int \frac{\rho(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|} d\mathbf{r}'$

PHYSICS QUANTITIES

The simulated input is an output of another model, as defined in the workflow.

3. SOLVER AND COMPUTATIONAL TRANSLATION OF THE SPECIFICATIONS

NUMERICAL SOLVER: Iterative Self-consistent eld (scf) eigensolver for DFT problem Davidson or Conjugated gradient - electronic structure BFGS quasi-newton algorithm - optimization of atomic structure

SOFTWARE TOOL: Quantum-Espresso (QE) (QE, www.quantum-espresso.org) and SIESTA (www.icmab.es/siesta)

TIME STEP: N/A

COMPUTATIONAL REPRESENTATION

PHYSICS EQUATION: DFT problem is solved for a set of valence electrons corresponding to the atoms in the simulation cell. Kohn-Sham equation is represented in the matrix form. Eigenvectors (eigenvalues) of KS equation are the single particle wavefunctions (energies) of the matrix problem. Monkhorst-Pack mesh is used for Brillouin zone sampling and k-summation.

MATERIAL RELATIONS: Single particle KS orbitals and charge density are expanded on plane-wave basis set in QE or finite-range pseudo-atomic orbital (PAO) in SIESTA. Charge density and potential are calculated on FFT grids.

MATERIAL: Nuclei are represented by points in the real space, whose charge is defined by the corresponding pseudopotential.

COMPUTATIONAL BOUNDARY CONDITIONS: Periodic boundary conditions

ADDITIONAL SOLVER PARAMETERS: Atomic structures are relaxed until forces on all atoms become lower than 0.03 eV/Ang-1. Kinetic Cut off and PAO basis set depend on specific material simulation.

4. POST PROCESSING

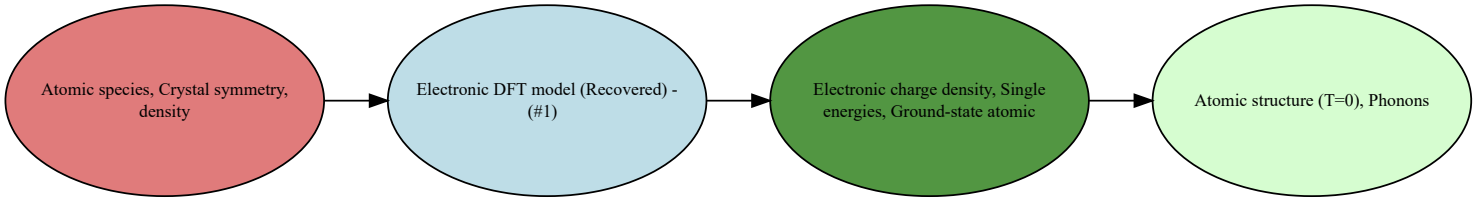
THE PROCESSED OUTPUT: Atomic structure (T=0), Phonons

METHODOLOGIES: Phonon are calculated in the linear response approximation through the resolution of the Stemmeimer equation.

MARGIN OF ERROR: Margin of error: ~ 10%. Mostly due to the error in the material relations (e.g. exchange and correlation functionals).

MODA WORKFLOW PLOT

Note: long text may not be displayed in full


Atomic species, Crystal symmetry, density
Electronic DFT model (Recovered) - (#1)
Electronic charge density, Single energies, Ground-state atomic
Atomic structure (T=0), Phonons