DEEPEN

From atom-to-Device Explicit simulation Environment for Photonics and Electronics Nanostructures

www.nmp-deepen.eu

A MULTISCALE OPEN SOURCE SOFTWARE ENVIRONMENT FOR THE SIMULATION OF ELECTRONIC AND OPTOELECTRONIC DEVICES

DEEPEN is funded by FP7 under NMP-2013-1.4-1 call with Grant agreement no: FP7-NMP-604416

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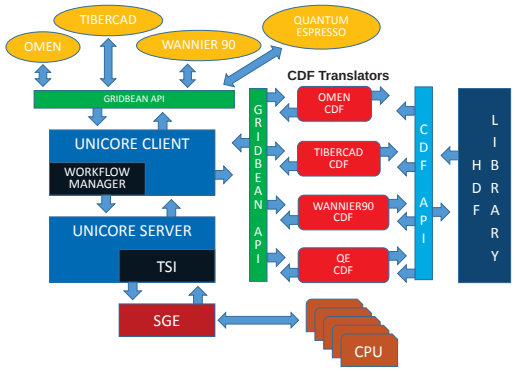
ABSTRACT

We present the main results of the FP7 Project **"From atom-to-Device Explicit simulation Environment for Photonics and Electronics Nanostructures"** (**DEEPEN**). The aim of the project is to develop an Open Source software environment for the **multiscale** simulation of electronic and optoelectronic devices. In particular it is focused on the predictive design of novel materials and nanostructures, such as LEDs based on InGaN/GaN nanowires (NWs) and InGaN/(Al)GaN quantum wells (QWs), as well as nano-scale electronic devices including new channel materials, such as InGaAs, for sub-10 nm CMOS. The Multiscale **Open Source Interface (OSI)** is designed to be **flexible** and **extensible** to a wide range of simulation codes. To satisfy these requirements, it is based on the **UNICORE** OS grid middleware for access to modern heterogeneous computer networks. In this framework, complex simulation protocols, including multiple steps to treat different size scales, can be implemented in the form of extendable generic **workflows**.

The software tools employed for multiscale simulations in this project implement physical models at different scales, ranging from ab-initio Density Functional Theory (**DFT**) and Empirical Tight-Binding (**ETB**) at **atomistic** scale to **Drift-Diffusion** at **continuous** scale. They have been integrated in the **OSI** through the **UNICORE APIs,** which allow to exchange data of different kind between the simulation tools while keeping them separated from the platform. An open source Common Data Format (**CDF**) based on the **HDF5** standard allows for **interoperability** betweeen the different simulation tools. Widgets called **CDF Translators** act as translators between each tool's proprietary format and the CDF. Different types of multiscale models have been implemented to link simulations at different scale. A ***parametric linking*** allows the extraction of material parameters from ab-initio (DFT) calculations for use in Tight-Binding and Drift-Diffusion simulations of QWs and NWs. Based on this, a **material database** has been obtained for nitrides and III-V systems. A ***DFT/Tight-binding linking*** is used to perform quantum transport calculations in InGaAS NWs and channel devices through Non-equilibrium Green Function (NEGF) models, based on ab-initio Hamiltonians. Finally a ***self-consistent coupling*** between **NEGF** quantum transport and Drift-Diffusion is implemented in a commercial tool (**Synopsys S-Device**).

MULTISCALE OPEN SOURCE INTERFACE (OSI)

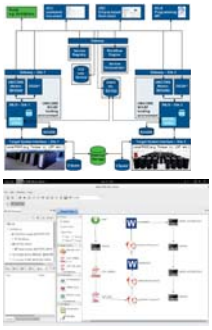


Flexible and Extensible OSI

- ***Extension*** of the OSI with a new tool requires no modification to its code, but only implementation of Unicore APIs.
- Use of a CDF allows for ***flexible*** linking through the tools, facilitating exchange of data.

OSI Implementation in Unicore

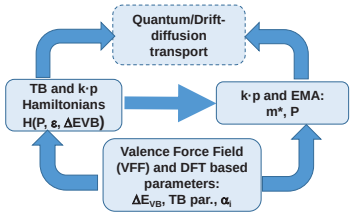
- **Based on the UNICORE standard**
  UNICORE (www.unicore.eu) is an European project that facilitates the access to modern heterogeneous computer networks. It is a standards-based complete Grid middleware stack which offers a client-server framework for accessing Grid resources. Main features: Open Source project, Java based, supports common operating and resource management system, Open and extensible (Service Oriented Architecture).
- **Common Data Format (CDF)**
  An **HDF-based** open source Common Data Format (CDF) allows interoperability betweeen different simulation tools. HDF features allow the exchange of solution quantities of any kind and the specifications of complex data relationships and dependencies. Widgets called **CDF Translators** act as translators between each tool's proprietary format and CDF. CDF translators allow to separate application tools from the platform; thus, in case of a new version of the tool only the CDF Translators need to be updated.
- **UNICORE APIs: GridBeans**
  Allow to exchange data while keeping application tools separated from the platform. A **Gridbean** is a widget in the workflow system, for the input and output data specifications and the configuration for grid services, together with an optional interface for interacting jobs.
- **Definition of simulation workflows**
  Simulation tools, implemented as widgets, are then combined in a **Workflow** to execute multiscale couplings schemes.
- **Material parameters database**
  Implemented with HDF files, is able to contain binary data in a hierarchical structure and allows direct access to parts of the file without first parsing the entire content.



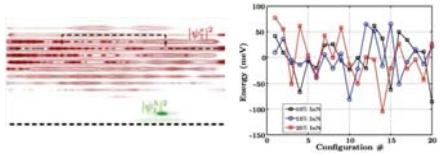
- **Control of Simulation Flow** implemented using UNICORE clients for workflow generation.
- UNICORE Graphical Client (**URC**) based on **Eclipse** framework, easy **extensibility** via plugins.
- An UNICORE generic **Workflow** is composed of calls to individual applications (**jobs** to be executed) and control structures.

PARAMETRIC LINKING

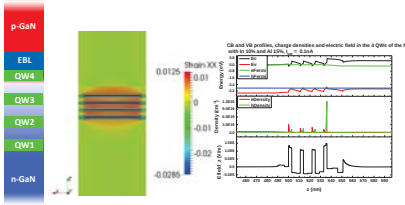
Extraction of parameters from ab-initio (DFT) for linking to Tight-Binding and Drift-Diffusion



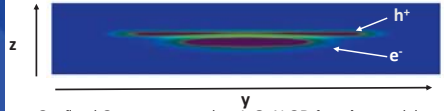
Tight-Binding Calculations for InGaN/GaN QWs: Localization Effects due to random alloy fluctuations



Parametric linking: tight-binding material parameters used in continuum models for InGaN/GaN NWs



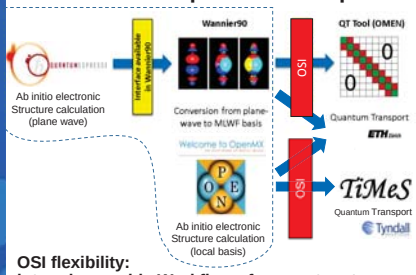
Strain map, band profiles and particle densities in 4QD-NW



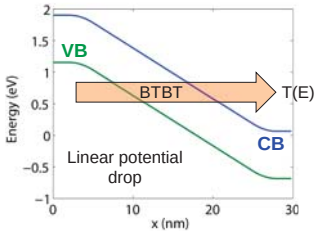
Confined Quantum states in a InGaN QD from **k·p** model

DFT/TIGHT-BINDING LINKING

Ab-initio to quantum transport model

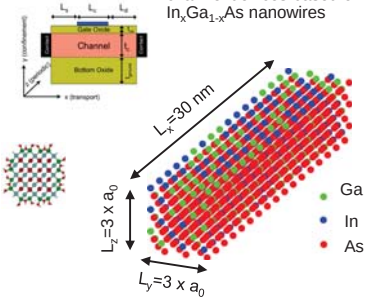


OSI flexibility: inter-changeable Workflows for quantum transport with different simulation tools

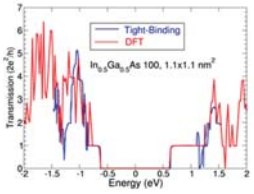


Calculation of the Band-to-Band Tunnel (BTBT) transmission T(E)

Transport simulations in channel devices based on $In_xGa_{1-x}As$ nanowires



Generation of $In_xGa_{1-x}As$ nanowires based on random alloy 3x3 supercells $In_xGa_{1-x}As$



Transmission for [100] InGaAs NWs calculated using TB and DFT

TIGHT COUPLING – NEGF/DRIFT-DIFFUSION

- Coupling of NEGF to Drift-Diffusion models
- **Self-consistent** coupling of Synopsys Sentaurus-Device to **quantum transport tools** (e.g. OMEN) for transport simulations
- Application to nano-scale transistor with InGaAs channel: source-drain tunneling, device optimization.