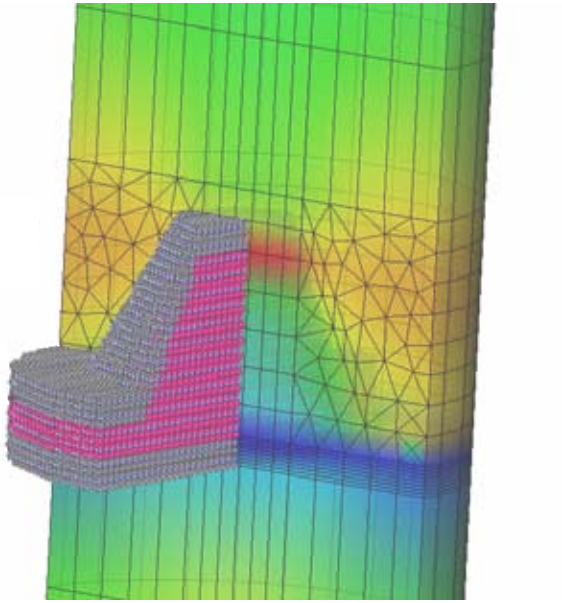
# tiberCAD
multiscale simulation

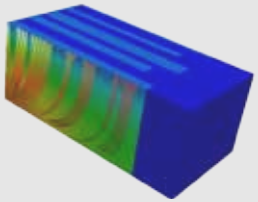
***tiber*CAD** is a software solution for the multiscale simulation of nanostructured electronic devices for applications in organic and inorganic optoelectronics, sensors, energy harvesting. ***tiber*CAD** allows the simultaneous solution of physical models on different length scales, ranging from FEM continuous models to atomistic descriptions. Quantum models may be coupled with classical solutions for applications in particle transport, electronic properties, heat dissipation, mechanical deformation. Examples of use are atomistic modelling of alloy fluctuations in Nanowire and Quantum Well-based LEDs, simulation of organic and inorganic solar cells, NW-FETs, piezoelectric nanogenerators.

***tiber*CAD** provides innovative design and analysis tools to accomplish the critical requirements imposed by the recent developments in nanotechnologies.



## Dye Solar Cell

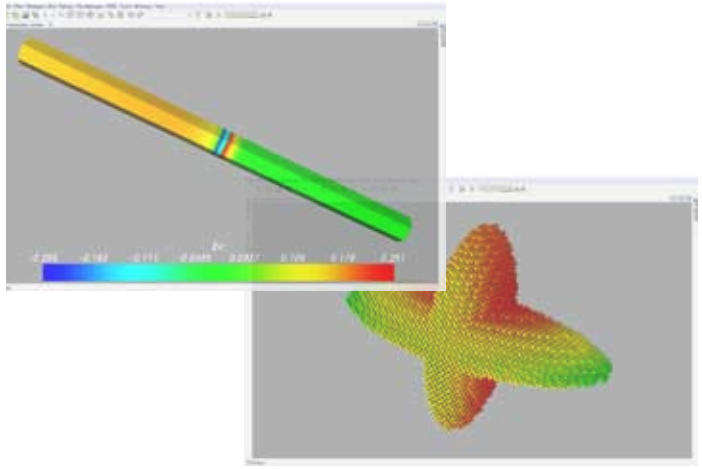
DSC



A finite element based electrical model of a **DSC**. The module allows the modeling of a complete **DSC** (including porous material, electrolyte region and contacts) with generic geometry and dimension (1, 2 and 3D). User-defined dyes and source spectrum can be employed. Different parameters, for the electron recombination and charge carrier mobility, can be set.

### Main Features

- Modeling of the entire cell in 1, 2 and 3D
- Several dyes available
- Inclusion of traps
- Visualization of all charge carriers, currents and densities

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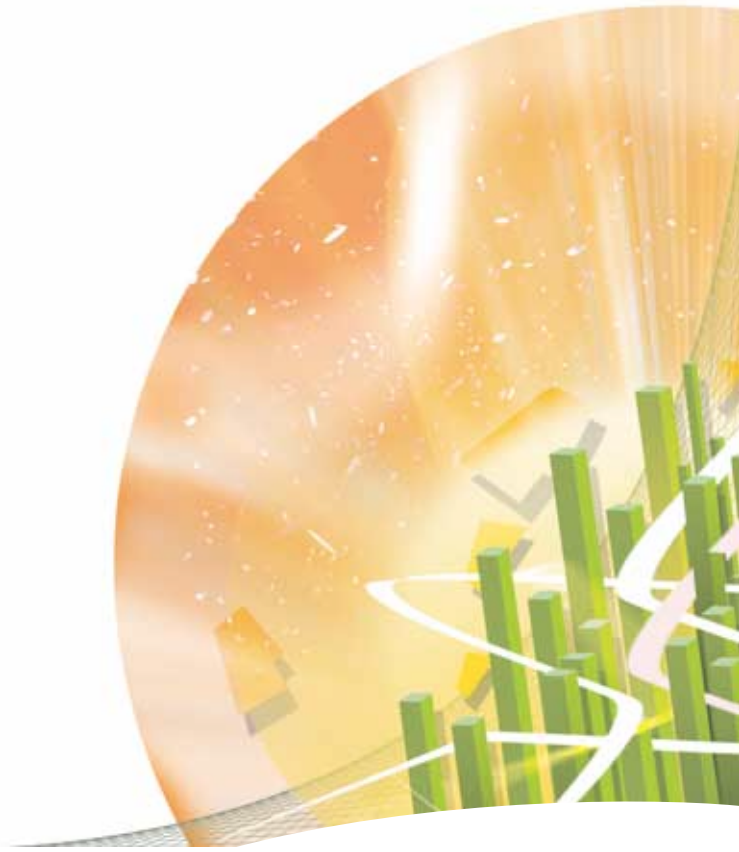
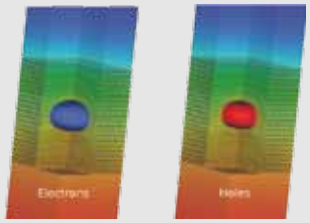


*a software developed by*

tiberlab

## Drift-Diffusion

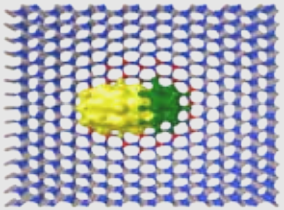



Transport of electrons and holes is calculated based on the **Drift-Diffusion** approximation. Mechanical, thermal and quantization effects can be included self-consistently by coupling to the **Elasticity**, **Thermal** and **Envelope Function Approximation** modules.

### Main Features

- Models for transport in organic devices: Gaussian DOS, Hopping mobility model
- Accounts for full strain tensor and piezoelectric field
- Band parameters based on strain corrected bulk **k•p** model
- Easy coupling to Thermal, Elasticity and EFA modules

## Atomistic

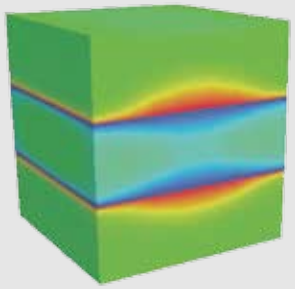


Atomistic models for quantum calculation of electronic and optical properties of nanostructures with Empirical Tight Binding (ETB). Combined with a built-in atomistic generator and a structure relaxation tool based on Valence Force Field (VFF), it allows to treat in a fundamental way nanometric features in Quantum Well and Quantum Dot active regions, such as alloy fluctuations. Random alloy representations provide a realistic picture of an LED active region.

### Main Features

- Built-in Atomistic generator
- Supports VCA and random alloy approach
- Atomic structures from external files
- Accurate ETB $sp^3s^*d^5$ parameterization, including GaN/AlGaN/InGaN systems
- Full examples of Nanowires and Quantum Wells for applications in photonics

## Elasticity

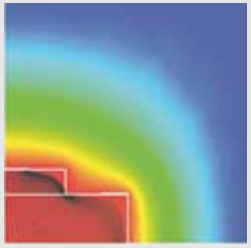


**Elasticity** brings features developed for continuous elasticity into device modeling. The coupled treatment of the electro-mechanical problem allows to explore the feasibility of devices where the mechanical deformation plays a fundamental role.

### Main Features

- Continuous elasticity
- Converse piezoelectric effect
- Isotropic and anisotropic stiffness tensor
- Lattice mismatch induced strain
- Application of an external surface force

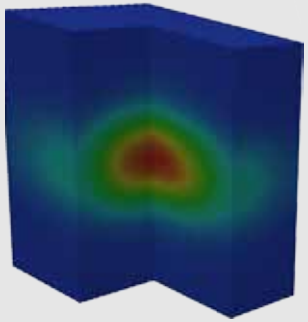
## Thermal



**Thermal** provides the temperature maps obtained by the balance between the Fourier heat transport and the Joule heat. The deep integration with **Drift-Diffusion** makes **Thermal** a powerful tool for thermal analysis of devices

### Main Features

- Fourier heat transport
- Electrons and holes Joule and recombination heat
- Peltier effect
- Anisotropic thermal conductivity



Quantum calculations in the framework of **Envelope Function Approximation (EFA)**. The solution of the eigenvalue problem provides eigenstates and eigenfunctions of the system, particle densities and optical emission spectrum.

## Envelope Function Approximation

### Main Features

- Modeling of 1, 2 and 3D structures: quantum dots quantum wires, NWFETs
- Zincblende and wurtzite crystalline structures fully supported including strain correction
- Single band and multiband 6x6, 8x8 **k•p** model
- Self-consistent Schrödinger/Poisson simulation