Multiscale Modelling Made Simple – “NanoBridge”- A Computational Platform for Next-Gen Simulations of Novel Devices incorporating 2D materials.

The demand for electronics is exponentially increasing, electronic devices continue to shrink in size-while at same time are required to deliver better performance and expanding functionality, furthermore, these devices also require exponentially more power to operate. Incorporating the use of novel 2D materials with unprecedented properties could provide a response to this challenge.

When numerically studying the performance of devices incorporating 2D materials, the primary hurdle lies in addressing the extreme geometrical aspect-ratio between nanostructured materials and device environments, the low dimensionality of the materials and the coexistence of multi-physics phenomena involving electromagnetism (EM), charge propagation, heat transfer, amongst others. The use of this multi-physics (multiscale) toolkit provides high predictive capabilities and is a source of helpful information to manage and direct the design and manufacturing phase of the devices

The computational platform offers simulation engines covering the entire range of atomic-scale simulation methods for the materials and subsequently devices of interest which develops and integrates:

1. ab-initio simulations at atomistic level
2. Monte Carlo simulations at meso-scale level
3. full-wave simulations at continuum level.

The *in-silico* approaches that are included in the platform complement each other: for successful use of atomic to meso-scale modelling, it is essential to have easy access to all the methods to combine them. Many different developed software packages are focused on one or some calculation methods, for this reason the development of a massive computational platform based on different tools has required a large effort for compilation, installation, and learning the input/output syntax. The tools are not fully compatible with any other packages, then learning the additional syntax within modelling class has required another large effort. Moreover, a single simulation tool method does not have all the required capabilities for the purposes of NanoBridge; hence, several different tools within each modelling class needed to solve a given problem, and a significant effort has been invested to master each of them. We have developed a computational tool based on different simulation engines, covering the entire range of atomic-scale simulation methods, then reaching full wave simulations.

In detail, we will use atomistic modelling and simulations to provide information about chemical-physical phenomena and to obtain constitutive relations to be included in simulators at the continuum level, to refine the calculation and to achieve truthful and reliable results. This means that *the architecture of our computational platform is based on a bridge between the discrete and continuous levels* (**Figure 1**).

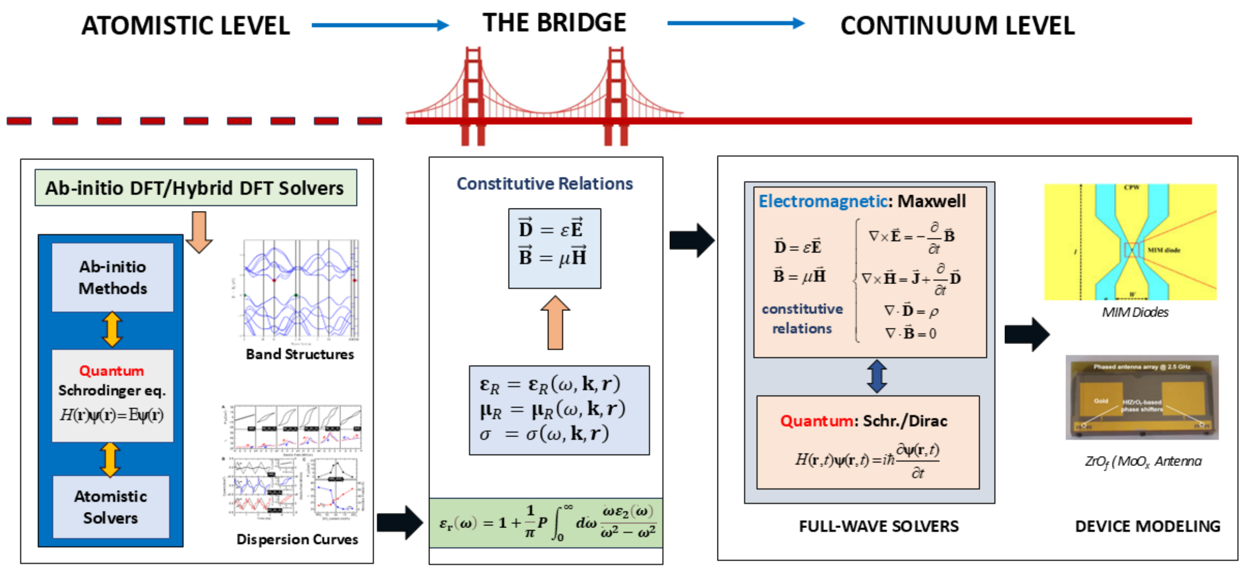

Figure 1: Description of NanoBridge Multiphysics platform. The different levels of theory are reported to highlight the connection point between discrete and continuum simulations.

At the atomistic level, the entire range of atomic-scale simulation methods is included, moving from near-exact quantum mechanical calculations to approximate simulations, and we will choose the best method to use in relation to the effect to investigate. The basic concept is that the in-silico approaches included in the platform complement each other: for successful use of atomic to meso-scale modelling, it is essential to have easy access to all the methods to combine them. For this reason, we use Density Functional Theory (DFT) as the most important first principle computational method, including corrective terms if necessary, and compiling parameter files for semi-empirical calculations (**Figure 2**).

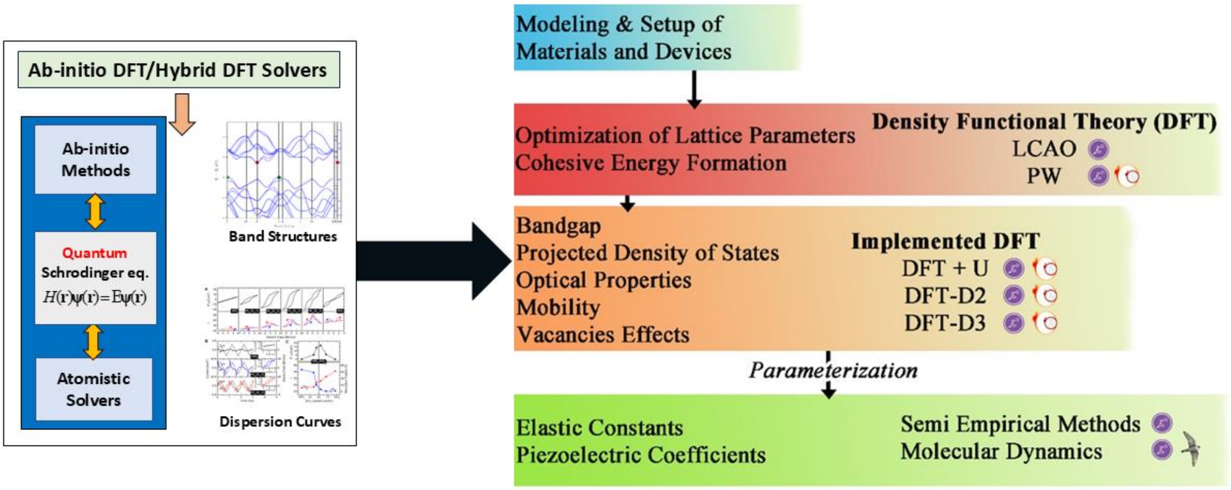

Figure 2: Description of computational platform. The purple icon is referred to the possible use of Quantum Atomistic ToolKit (Q-ATK) software, while the white and red symbol remarks the possibility to use QuantumEspresso (QE) package; the hawk icon highlights the possible use of Gromacs software.

More in detail, Quantum Atomistic ToolKit (Q-ATK) [1] represents the most important software used inside the proposed computational platform. It is a released software with licenses that allows generating simulations models through its modern graphical user interface (GUI). It includes many different simulation methodologies required, and all the computationally demanding modules may be run in parallel on many processors at once, using message passing between processes and/or shared-memory threading and in a multi-level approach. Another software adopted is Quantum Espresso (QE) [2], which is an integrated suite of Open-Source computer code used inside the platform. The graphics processing unit (GPU) accelerated version of this suite is installed on High Performance Computing (HPC) Center at Cineca ISCRA platform in Casalecchio di Reno [3] (Bologna, Italy), and the acceleration is the most important advantage in the use of QE by remote way. Using the same input/output syntax, we have modelled atomistic systems and carried out computational methodologies using Q-ATK, then each input file has been accompanied by a command file to direct the simulation in QE. With the Q-ATK-QE linkage we have simultaneously conducted many different calculations leveraging both local computing resources and remote computing clusters. Another part of our computational platform is represented by GROMACS, a versatile package [4] able to perform molecular dynamics (MD) simulations for systems with hundreds to millions of particles. This software is a free licensed package which includes many different force fields as LAMPPS [5] and CLAYFF [6] that can be implemented with parameters obtained through other investigations based on other computational suites. Our approach is to use Q-ATK and QE to obtain precise parameterizations for materials of interest and then to simulate their properties using the force field (FF) and semi empirical (SE) methods. Still concerning GROMACS, a GPU accelerated version is installed on HPC Cineca platform (*vide supra*), then we have performed high extensive simulations obtaining results in a very reasonable time. The computational platform includes the most important FF packages implemented with empirical evidence but, more importantly, the predefined literature parameter sets can be invoked from the NanoLab GUI included in Q-ATK. It is also possible to specify custom FF parameters via the Potential Editor tool in a Python script from Q-ATK and QE to implement FFs included in GROMACS. This way, we have carried out fast simulations including a high number of atoms, decreasing the accuracy degree and maintaining high reliabilities thanks to the refined parameters.

In reference to the computational methods, the starting framework of our platform for *ab initio* electronic-structure theory is represented by DFT, which provides computationally tractable solution to the electronic manybody problem and gives high predictive power with respect to experiments [7]. The exchange correlation (xc) functional is the only formal approximation in DFT approach, since the exact functional is unknown. Our platform supports a large range of approximate xc functionals including the local density (LDA) and generalized gradient (GGA) approximations. Furthermore, the computational platform supports spin-unpolarized and spin-polarized (both collinear and noncollinear) variants for each xc functional. All DFT results are based on the use of GGA functionals [8] which assume that the exchange and the correlation energy in a point depends not only on the density in that point, but also on its gradient of electron density following the equation (i):

$$ExcGGA\,[n] = \int n\,(\boldsymbol{r}) \in xc(n(\boldsymbol{r}),\ |\nabla n(\boldsymbol{r})|)\ d\boldsymbol{r} \tag{i}$$

In which the term $|\nabla n\,(\boldsymbol{r})|$ is the addition for the gradient, and the density $n\,(\boldsymbol{r})$ represents the number of electrons per unit volume.

In periodic systems a given element may be present in different spatial arrangements displaying vastly different physical and chemical properties; for this reason, an elemental basis set that is independent of physical properties of materials may lead to significant simulation inaccuracies. To avoid such a lack of material specificity within a given basis set, it is of crucial importance to choose between different basis set to better represent the shapes of orbitals and then to simulate the correct wavefunctions overlapping. For this purpose, inside our platform DFT is implemented with the linear combination of atomic orbitals (LCAO) and the plane-wave (PW) basis set approaches, and both are obviously combined with different pseudopotential methods. DFT-LCAO can be used with Q-ATK software, and it represents an efficient implementation for layered materials, interface structures, models with vacancies and, in general, for systems with mixed boundary conditions [9]. For this formalism, the single-electron eigenfunctions, ψ_α, are expanded in a set of finite-range atomic-like basis functions φ_i following the equation (ii):

$$\psi_\alpha\,(\boldsymbol{r}) = \sum_i c_{\alpha i}\,\varphi_i\,(\boldsymbol{r}) \tag{ii}$$

The use of all electron LCAO calculations allowed us to accurately describe the electronic distributions both in the valence and in the core region with a limited number of basis functions. The local nature of the basis allows a treatment both of finite systems and of systems with periodic boundary conditions in one, two or three dimensions.

On the other hand, the plane-wave (PW) representation implemented in the platform is ideally suited for bulk configurations with periodic boundary [10], and it can be used with Q-ATK and QE. In this case eigenfunctions are expanded in terms of PW basis functions following the equation (iii):

$$\psi_\alpha (\mathbf{r}) = \sum_{|\mathbf{g}|<gmax} c_{\alpha,\mathbf{g}}\, e^{i\mathbf{g}\mathbf{r}} \tag{iii}$$

where α denotes both the wave vector k and the band index n, and g are reciprocal lattice vectors. The upper threshold for the reciprocal lattice-vector lengths included in the PW expansion (*gmax*) is determined by a kinetic-energy (wavefunction) cutoff energy E_{cut} with the equation (iv):

$$\frac{\hbar^2 g_{max}^2}{2m} < E_{cut} \tag{iv}$$

PW methods are the most popular in periodic systems calculations. Plane waves are an orthonormal complete set, where any function belonging to the class of continuous formalizable functions can be expanded with arbitrary precision in such a basis set.

Since DFT is well known to reproduce the steady-state properties of materials in an accurate way, the purpose of the NanoBridge simulation approach is to investigate the excited state phenomena with the aim to predict the physical-chemical behaviour of the studied materials. Moreover, the inclusion of polyelectronic atoms such as Hf, Zr, Mo, and V leads to some important effects that must be considered in the simulations and that are not correctly described by canonical DFT approach. One example is the inclusion of the strong on-site Coulomb interactions of localized *d* and *f* electrons involved in the chemical bonds, as for Hf, Zr, and V. We have described these repulsive terms adding a Hubbard corrective term DFT approach following the equation (v):

$$E_U = \frac{1}{2}\sum_l U_l (n_l - n_l^2) \tag{v}$$

where n_l is the projection onto an atomic shell l, and U_l is the Hubbard U for that shell. The energy term E_U is zero for a fully occupied or unoccupied shell, but positive for a fractionally occupied shell. This method is called DFT+U [11] and can be adopted with both LCAO and PW basis set.

Another important example of effects that need to be reproduced is represented by the van der Waals dispersions for layered materials, as for MoS_2. In this case, both DFT-LCAO and DFT-PW methods can be implemented with two-body and three-body dispersion corrections by Grimme with approaches called DFT-D2 [12] and DFT-D3 [13], respectively. For the first method, we have added a pair-wise atom-atom potential to the DFT approach following (vi):

$$\frac{C_{6,iJ}}{r_{iJ,L}^{6}} \tag{vi}$$

where $C_{6,ij}$ is the dispersion coefficient obtained by DFT calculations of polarizabilities and ionization potentials of the isolated atoms, while $r^6_{ij,L}$ is the distance between the atoms as a function of the translation in the unit cell L. Another dispersion correction method for density functionals is DFT-D3, which is a refined version of DFT-D2. The biggest difference with its predecessor is that its dispersion coefficients are fully flexible and system dependent. For this reason, the C_6 terms are no longer scaled, and the higher C_n terms are necessary to adapt the potential specifically to the DFT approach adopted.

Since only the outermost electrons determine the formation of chemical bonds with other atoms, with the aim to approximate the effects of core electrons avoiding explicit DFT calculations of core electrons, our platform uses pseudopotentials (PPs) and currently supports both scalar-relativistic and fully relativistic normconserving PPs [14]. The computational platform is shipped with built-in databases of well-tested PPs covering all elements up to Z = 83 (Bi) and excluding lanthanides. The most useful PPs for our simulations are SG15 [15] and PseudoDojo [16] sets. These are two modern normconserving PP types with multiple projectors for each angular momentum, to ensure high accuracy. Both sets contain scalar-relativistic and fully relativistic PPs for each element.

Since the calculation of some properties of interest for the project require the inclusion of many atoms (e.g., for the mechanical properties of materials), other important approaches considered in the proposed computational platform are semiempirical (SE) methods and molecular dynamics simulations based on FF approach. The use of computationally fast alternatives to DFT as SE methods is related to the use of libraries with precalculated parameters. Our multi-software platform allowed us to generate specific packages to include in the SE calculation, avoiding self-consistent loops. In details, transport calculations for obtaining I-V characteristics curves and transmission pathways plots were all based on SE Tight-Binding (TB) approach [17] and Non-Equilibrium Green's Function (NEGF) formalism [18]. This method treats the effect of the external potential on the entire system (atomic and trench regions) with desirable computational efficiency and with quantitative agreement with experimental results as reported in the result section.

On the other hand, the FF approach is fully integrated in the Python framework, and then, as for the SE methods, the FF parameters can be implemented with DFT derived parameters. FF approach has allowed us to carry out MD simulations using empirical potential models. The simulation engine also allows to assign different FFs to different sub-systems. The empirical potential for each sub-system and the interactions between them can be customized as desired using Python scripting again. Our computational platform currently includes more than 300 predefined literature parameter sets, which can conveniently be invoked from the GUI and can be implemented using the approach that has been previously described for the SE implementation.

To give an idea about the computational cost of the different atomic-scale simulation methods included in our platform, the computational speed of the methods has been compared when simulating increasingly larger structures of HfO_2 (**Figure 3**).

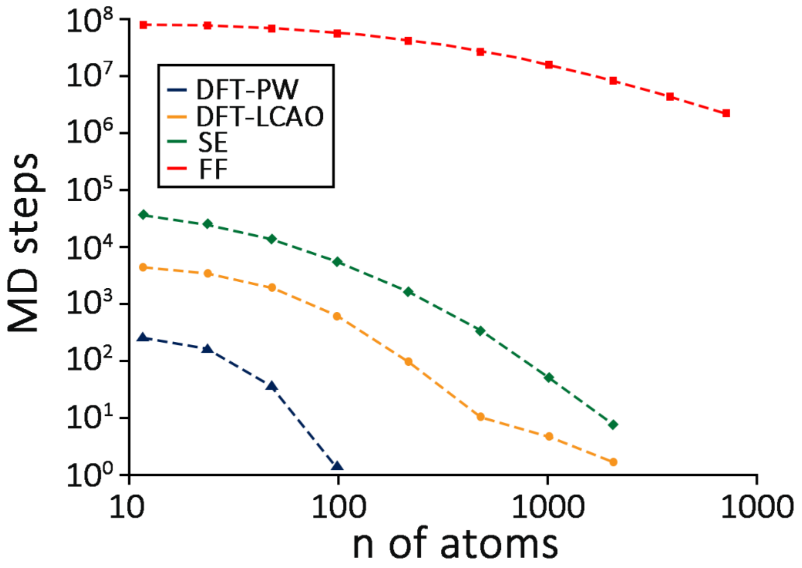

Figure 3: Comparison of the simulation methods available in our platform, considering the total number of molecular dynamics steps performed in 24 h (MD steps) against system size (n of atoms) of monoclinic HfO_2.

The measure of speed is referred to the number of molecular dynamics steps that are feasible within 24h when run in parallel on 16 computing cores. This comparison has been carried out on a 16-core central processing unit (CPU) of type Intel I9 10900K. The CPU times show that the PW approach is computationally demanding for higher systems, while the LCAO approach can be more than an order of magnitude faster for systems with more than 100 atoms.

Despite the high degree of accuracy achieved by using software in a combined way, materials can exhibit different chemical and physical properties depending on their specific dimensions and the circuit context in which they are located. Therefore, it is necessary to recreate the boundary conditions for each component in order to simulate an entire device. We now introduce the atomic-scale methodology used in simulated devices. All the simulations have been performed again with Q-ATK software, using SE method [19],[20] implemented by tight-binding (TB) calculations. From our knowledge, Q-ATK is the unique atomistic software with the capabilities of modelling the concept devices. Firstly, the modelling of devices such as Metal-Insulator-Metal (MIM), self-switching (SS) or geometric diodes must be performed using the previously optimized structures as single monolayers and discrete sized systems, then the non-equilibrium Green's function (NEGF) will be used to

calculate the self-consistent device potential and charge distribution [21], [22]. The multi-grid Poisson solver is the adopted approach to predict the Hartree energy by solving the Poisson's equation. Meanwhile, the non-self-consistent part of the tight-binding Hamiltonian will be parametrized using Slater–Koster model in which the distance-dependence of the matrix elements is given as a numerical function [20].
Once the self-consistent non-equilibrium density matrix will be obtained, the transport property and current amount of graphene devices have been calculated by using transmission coefficient T at electron energy E determined from the retarded Landauer formula (vii) [23]:

$$\mathrm{I}(V_L T_L V_R T_R) = \frac{e}{h}\sum\int T_\sigma(E)\left[f\left(\frac{E-\mu_R}{K_\beta \mathrm{T}_R}\right) - f\left(\frac{E-\mu_L}{K_\beta \mathrm{T}_L}\right)\right] dE \tag{vii}$$

Where f is the Fermi energy, T_L/T_R is the electron temperatures of the left/right electrode, and $T_\sigma(E)$ is the transmission coefficient for the spin component σ. Meanwhile, the chemical potentials of the right/left electrode and V_{bias} can be defined by Equations (viii-xi) (2-5):

$$\mu_R = E_F^R - eV_R \tag{viii}$$

$$\mu_L = E_F^L - eV_L \tag{ix}$$

$$\mu_R - \mu_L = e\,V_{bias} \tag{x}$$

$$V_{bias} = V_L - V_R \tag{xi}$$

Beginning with the outcomes of the DFT simulations (e.g., band structure, charge wavefunctions, etc.), a rigorous process rooted in the Kubo-Greenwood formalism is utilized to incorporate the quantum properties of materials into electromagnetic (EM) constitutive relations [24]. This integration enables precise and rigorous EM simulations of complex devices. EM solvers, whether commercial or in-house, typically include databases containing information on all known materials. However, these databases inevitably lack the permittivity and permeability data for novel materials. Computing these parameters for novel materials presents a significant challenge and was among the most noteworthy scientific advancements of our computational platform [25].

At the meso-scale level, a very advanced Monte Carlo (MC) solver has been developed that is particularly effective for studying devices subject to drift diffusion phenomena. MC is a numerical method used to study carrier transport in electron devices by solving the Boltzmann equation rigorously [26]. Typically, it is combined with Poisson's equation to ensure self-consistency. MC allows us to analyse the electrical properties of devices with dimensions in the hundreds of nanometres range. Unlike quantum transport simulators such as the NEGF method, MC can handle these relatively large dimensions that are too computationally intensive for the former. We have been able to enhance prior MC simulations [27] by developing a code that couples charge motion with a rigorous solution of Maxwell's equations in the time domain instead of Poisson's equation. This approach enabled us to study the transient behaviour of devices and accurately characterize their electrical performance at high frequencies, including in the terahertz (THz) range or infrared (IR) range.

The MC simulator complements electromagnetic simulators like COMSOL or HFSS and allows for numerical evaluation of electrical properties of proposed devices, such as I-V characteristics and impedance, crucial for designing very high-frequency devices. Examples applications are its use to assess the high-frequency impedance of rectifying diodes, facilitating proper matching with antenna impedance when designing rectennas.

For the full wave simulations at continuum level the following approach was used. After accurately evaluating constitutive equations and relations, ab initio simulations at the atomistic level were used to incorporate material properties into larger scale models. This process enabled us to include all necessary physics in full-wave simulations at the continuum level.

These simulations are carried out using tools that combine available electromagnetic solvers such as COMSOL, HFSS, and CST, with custom solvers designed to solve systems of partial differential equations, including those related to charge transport phenomena based on either the Maxwell-Schrödinger or Dirac/Boltzmann equation solutions [28].

In Figure 4 below we present the semantics and the development of the entire computational architecture. In summary, computational tools are organized (and can be viewed) in three main blocks:

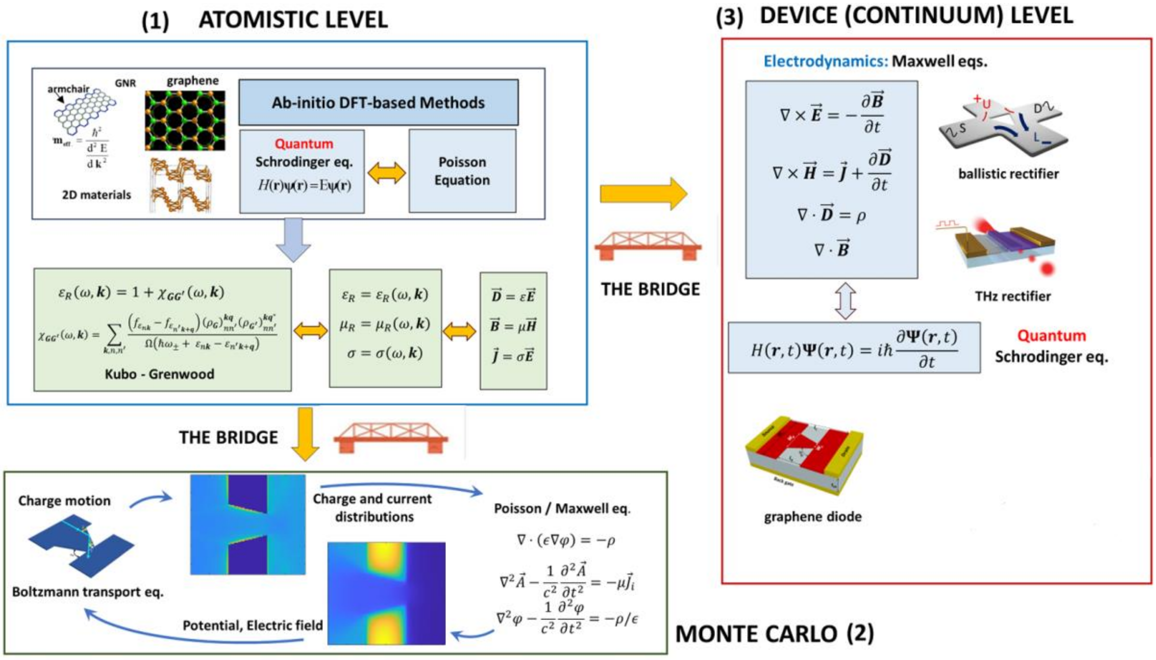

Figure 4. Semantics and the development of the computational architecture

In block (1) on the left-top side the chain of tools for the ab initio calculation, defined atomistic level simulations as they act on discrete and sometimes very complex domains, as atoms, aggregates of atoms or molecules of the material.

In block (2), MC is illustrated. Charges traverse a patterned graphene domain under the influence of an electric field, resulting in surface charge densities and currents. These produce an electromagnetic field, governed by either the Poisson or Maxwell equations in steady-state or time-varying domains, respectively. The resulting electric field, in turn, influences the motion of charges.

Block (3), shows modelling and simulations of electrical/electronic systems over the whole EM spectrum, founded on the implementation and solution of Maxwell equations.

The key development is the bridge from atomistic-to-continuum level, as it permits to construct the material permittivity, permeability, and conductivity to be used in (2) and (3). These relations incorporate the atomistic description of the field-matter (material) interaction but translate it to the meso-, macroscopic, phenomenological level, by means of permittivity, permeability (and/or conductivity) of the material(s).

In other words the computational platform offers simulation engines covering the entire range of scale moving from near-exact quantum chemical calculations to approximate continuum simulations.

The evolution of future radio mobile networks 6G or high responsivity sensors for example, demand the integration of increasingly eco-friendly, CMOS-compatible, ultra-fast transient response, electrically tunable, and low-consumption devices. The modelling platform mentioned above can be used to address the challenges faced in designing these novel devices making use of 2D materials.

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