European Cooperation in Science and Technology (COST) is a funding organization for the creation of research networks, called COST Actions.

EsSENce Cost Action CA19118

Project Title:

"High-performance Carbon-based composites with Smart properties for Advanced Sensing Applications"

Deliverable No	D5.2
Deliverable Title	REPORT/ARTICLE IN SIMULATION METHODOLOGIES FOR PROPERTIES/RESPONSES PREDICTION OF CNM COMPOSITES
Working Group	WG5 - DESIGN THROUGH COMPUTATIONAL MODELLING
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Table of Contents

Table of Figures

1 Introduction

In EsSENce, WG5 covers the materials and sensing mechanisms modelling, identified as a key area to support the development of carbon-based nanomaterials (CNMs) and advanced high-performance composites, and their implementation into products. In this sense, the working group is expected to promote i) the use of “standard” or widely agreed modelling protocols, or ii) the development/application of new modelling approaches. In addition, WG5 aims to be a forum to identify the needs in this field considering both experimental characterization (needed to feed or validate the models) and modelling points of view. Finally, other objectives of this group include disseminating design practices, to assess their applicability in industrial environments and to develop educational material in order to spread them as much as possible in the large community dealing with advanced high performance CNMs.

Two deliverables have been defined for WG5:

D5.1: Open Access Database – modelling results and contributions related with CNM composites for sensing applications.

D5.2: Report on simulation methodologies and methods for properties/responses prediction of CNM composites.

This report refers to the second one. However, it is worth mentioning that the deliverables are linked, since it has been decided to consider a similar structure of folders/sections in both. The objective of the report is to make a review of models/approaches commonly used to support the study and the design of carbon-based nanomaterials (CNMs), advanced high-performance composites and sensors or self-sensing materials obtained from them, identify the outcomes/results that can be obtained and the weaknesses and strengths of each simulation methodology.

2 Simulation methodologies for properties/responses prediction of CNM composites

Recent advances in analytical and computational modelling frameworks to describe the mechanics of materials on scales ranging from the atomistic, through the microstructure or transitional, and up to the continuum. The multiscale modelling of materials approaches relies on a systematic reduction in the degrees of freedom on the natural length scales that can be identified in the material. Connections between such scales are currently achieved either by a parametrization or by a 'zoom-out' or 'coarse-graining' procedure.

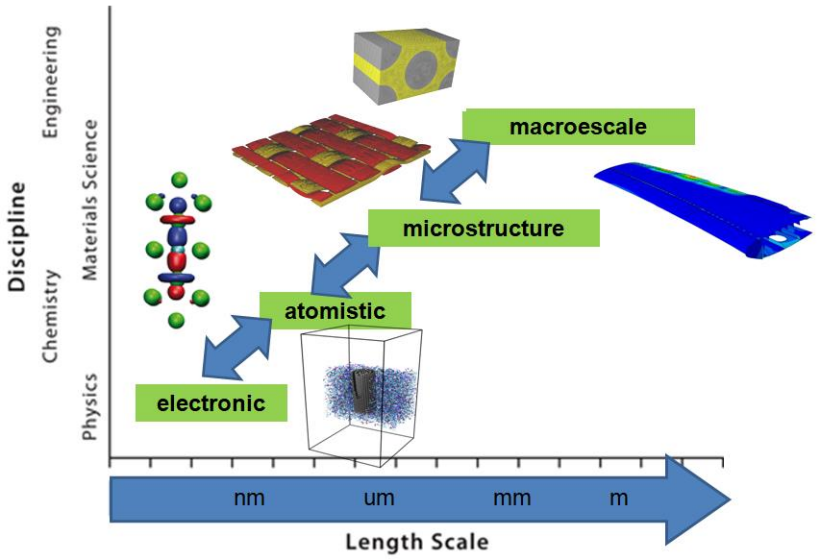

Figure 1: Multi-scale approach. Discipline vs. Length Scale.

Model	Entity whose behaviour is described	Number of entities	Indicative length scale (depending on current computers)	Indicative time scale (depending on current computers)
Electronic models	electron	10-100	0.1 - 1 nm	-
Atomistic models	atom	10^2 - 10^9	0.1 - 100 nm	fs - μs
Mesoscopic models	nanoparticle, grain, molecule, bead	10^6-unlimited	1 nm – 100 mm	ms - s
Continuum models	continuum volume	Unlimited (the model equations are written up for finite volumes or elements)	nm-m	s - ks

Figure 2: Models, entity, length scale and time scale [1].

This report presents a review of different modelling strategies and methodologies used within the framework of carbon-based nanoparticles (graphene, CNTs, nanofibers,….), CNMs and devices that can be obtained from this materials. Under this framework, the variety of models

and methods is extremely wide, and try to cover all of them in a report of reduced extension as the one proposed is almost impossible. Then, the review covers specific types of models and devices, generating the four main sections that constitute the document. The preparation of each section has been led by one WG5 member, specifically:

- Theoretical modelling of interactions of charged particles with graphene-based nanomaterials and their composites- Ivan Radovic.
- Molecular dynamics applied to CNM properties prediction - Matteo Fasano.
- Continuum micromechanics - Agustín Chiminelli.
- CNM devices - Graphene Field Effect Transistors - Alessandro Fantoni.

This review has been generated as part of the deliverables produced within the EsSENce CA, particularly from WG5.

2.1 Theoretical modelling of interactions of charged particles with graphene-based nanomaterials and their composites.

Graphene is the best known and the most explored two-dimensional (2D) material. It is the world's thinnest and strongest material, with the highest electrical and thermal conductivity known. Due to its outstanding physical, chemical, electrical and optical properties, graphene shows great potential in many fields, including sensors.

In nanoscale devices graphene typically appear in stacks separated by insulating layers of finite thickness [2][3][4], which usually support strong Fuchs-Kliewer (FK) or optical surface phonon modes [5]. Those phonon modes are active in the terahertz (THz) to mid-infrared (mid-IR) frequency range and can dampen the Dirac plasmon in doped graphene which operates in the same frequency range [6], or can hybridize with it [7]. As a prototype of layered nanostructures involving doped graphene sheets, members of this working group studied a graphene-sapphire-graphene composite system and found that the structure supports a variety of interesting plasmon-phonon hybrid modes in the THz to mid-IR frequency range [8]. The response function of graphene was obtained using two approaches within the random phase approximation (RPA): an ab initio method that includes all electronic bands in graphene and a computationally less demanding method based on the massless Dirac fermion (MDF) approximation for the low-energy excitations of electrons in the π bands. In our previous publication [9] we investigated the wake potential induced by an external charged particle that moves parallel to various sy_1-Al_2O_3-sy_2 composites, where the system sy_i (with i=1,2) may be vacuum, pristine (undoped) graphene, or doped graphene. Several important parameters were fixed at their respective typical values: the distance of the charged particle from the closest surface, the thickness of the sapphire (Al_2O_3) layer, and the doping density (i.e., Fermi energy) of graphene. In our recent publication [10] we presented a detailed study of the effects due to variations of all those parameters in the case of the wake potential (the total potential in the plane of the upper graphene sheet) produced by charged particle

moving parallel to the graphene-Al_2O_3-graphene composite system. In our very recent publication [11] we performed a thorough analysis of the stopping force (the dissipative force which opposes the particle's motion) and the image force (the perpendicularly oriented conservative force which bends the particle's trajectory towards the upper graphene sheet) on a charged particle moving parallel to the graphene-Al_2O_3-graphene heterostructure, covering broad ranges of the particle speeds and distances, as well as the doping densities of the two graphene sheets.

In all those publications, we considered an isotropic insulator (aluminium oxide, Al_2O_3) between two graphene sheets. We also assumed a zero gap between graphene and insulator to simplify calculations. Now we assign for the first time a finite gap size between graphene and insulator and examine the effects of the graphene-insulator distance on the plasmon-phonon hybridization. Besides, we explore the hybridization between the Dirac plasmon in graphene layer biased with a drift electric current and the surface optical phonon modes in the insulating substrate. We will also investigate for the first-time interactions of charged particles with two graphene layers separated by an insulating slab that exhibits anisotropy of a uniaxial crystal. An anisotropic layer of hexagonal boron nitride (hBN) will be chosen since van der Waals (vdW) heterostructures based on graphene and hBN layers with different stacking modes have attracting a great deal of interest because of their potential applications [12][13][14][15][16][17].

Electron energy loss spectroscopy (EELS) is a commonly used experimental technique for investigating electronic and plasmonic properties of materials, including (isotropic and anisotropic) vdW materials [18]. Members of this working group have extensive experience in the theoretical modelling of the experimental EELS data for free-standing (single and multilayer) graphene sheets obtained by scanning transmission electron microscope (STEM) [19][20], as well as in the theoretical modelling of the experimental EELS data for monolayer graphene supported by different substrates [21][22][23]. Now we derive a general expression for the effective dielectric function of multilayered materials made of 2D vdW materials separated by insulating layers, in order to obtain the EEL spectrum of such materials and compare it with the available experimental data.

Studying acoustic plasmons (APs) in single-layer, double-layer, and multilayer graphene or in metal/dielectric/graphene superstructures is a very active field of research. In our recent publication [24] we focused on the AP in graphene doped by alkali metals and demonstrated that two isoelectronic systems, KC8 and CsC8, support substantially different plasmonic spectra: the KC8 supports a sharp Dirac plasmon (DP) and a well-defined AP, while the CsC8 supports a broad DP and does not support an AP at all. These findings could be very useful in the area of chemical or biological sensing [25][26].

In our very recent publication [27] we used Kramers-Kronig analysis and ab initio calculations to develop a simple analytical method for including the effects of high-energy interband electron transitions in the density polarization function of doped graphene in the optical limit.

These results can be helpful in modelling and simulations of the THz spectroscopy of 2D materials [28] or in modelling vibrational spectroscopy of those materials in a monochromated TEM [29].

2.2 Molecular dynamics applied to CNM properties prediction

Classical Molecular Dynamics (MD) is a computational method to simulate the behavior of atoms and molecules over time. In an MD simulation, the trajectories of atoms (considered as rigid spheres) and molecules are determined by numerically solving Newton's equations of motion. Forces between particles are calculated exploiting calibrated interaction potentials (force fields), and from these forces, the accelerations, velocities, and subsequent positions of the atoms are determined [30]. For materials science, MD provides detailed insights into phenomena that might be difficult to observe directly, such as diffusion, phase transitions, interfacial effects, and the mechanical behavior at the nanoscale.

The essence of MD simulations lies in the force fields, which are mathematical models used to calculate interactions between atoms due to bonded or non-bonded interactions [31]. In MD simulations of CNMs, some specific force fields have gained prominence [32]:

- The Adaptive Intermolecular Reactive Bond Order (AIREBO) potential is tailored for carbon systems, capturing long-range van der Waals interactions and torsional effects. It is versatile for modelling both sp^2 and sp^3 hybridized carbon structures [33]. AIREBO might not perform well for systems with significant charge transfer or in case of interactions with elements outside its parameterization.
- Tersoff potential incorporates bond angles and lengths to offer a detailed representation of carbon interactions [34]. The potential may not be ideal for modelling weak interactions, and it might require recalibration for systems different from its original parameterization.
- ReaxFF is a reactive force field capable of simulating bond formation and breaking during MD simulations. This dynamic nature is achieved by not predefining specific bond types, allowing the system to evolve based on atomic positions and interactions. Due to its reactive nature, ReaxFF can be computationally demanding. It also requires careful parameterization for specific systems to ensure accuracy, e.g., in the case of condensed carbon phases [35].
- Machine Learning Interatomic Potentials (ML-IAPs) differ from traditional ones, as they do not depend on fixed mathematical formulas. Instead, they learn potential energy surface representations through training. Different implementations have been reported in the literature for certain carbon forms with near DFT-level accuracy, e.g., Gaussian approximation potential (GAP) [36], hybrid neural network potential (hNN-Gr_x) [37], GAP-20 potential for various crystalline phase carbon and amorphous carbon [38]. Despite the precision of current ML-IAPs in predicting properties of

carbon allotropes, challenges remain, especially regarding mechanical property predictions.

MD is suited for investigating various properties of CNMs [39]. *Mechanical properties* can be determined through MD simulations that simulate stress and strain [40]. In these tests, strain is applied systematically, and the resulting stress responses of the material are observed, providing data on its elastic constants, tensile strength, and potential fracture points [42]. However, these simulations face challenges, as the simulated strain rates should be much higher than those typically encountered in experimental setups to provide meaningful results in a feasible computational time. Another technique, nanoindentation, involves the simulation of a virtual indenter pressing into the material's surface, from which hardness and localized stress response can be derived [43]. The results, though, can be influenced by the chosen shape of the indenter and the interaction potentials utilized. *Thermal properties* of CNMs can be also explored using various protocols [45]. The Non-equilibrium Molecular Dynamics (NEMD) technique, for instance, establishes a temperature gradient within the simulation, enabling the calculation of thermal conductivity [46]. Still, it comes with the caveat that the artificially imposed gradient might not fully replicate real-world scenarios. The Equilibrium Green-Kubo method offers another approach, relying on the analysis of heat current fluctuations within an equilibrated system [47]. However, it often demands extended simulation times. Another critical thermal property is the thermal boundary resistance (TBR) [48]. As carbon nanomaterials are often interfaced with different materials (e.g., polymeric matrices, fluids), understanding the efficiency of heat transfer across these interfaces becomes vital [49]. The NEMD and Equilibrium MD protocols both offer quantitative insights into this property. Furthermore, theoretical models such as the Acoustic Mismatch Model and the Diffuse Mismatch Model, backed by inputs from MD simulations, provide complementary perspectives on TBR [54]. For *thermodynamic properties*, MD simulations lean on specialized techniques like free energy calculations. Advanced sampling methods, such as umbrella sampling and metadynamics, are employed to probe aspects like adhesion [55]. These methods require attention to force field choice and can be computationally intensive.

While offering mechanistic insights into the properties and behavior of CNMs, MD simulations are not without challenges, for instance:

- Temporal and spatial scales: MD simulations typically operate within specific temporal (fs to μs) and spatial (nm to μm) scales; phenomena outside these scales might not be captured effectively [57].
- Force field accuracy: The choice and accuracy of the force field can significantly impact the results. Not all force fields capture the intricate interactions in nanomaterials with equal fidelity [58].
- Computational cost: High-resolution simulations, especially those involving long timescales or large systems, can be computationally intensive, requiring substantial resources and time.

- Boundary conditions: The imposition of periodic boundary conditions can introduce artifacts, especially if the simulated system size is not sufficiently larger than the phenomena of interest [59].
- Thermal and mechanical loading rates: The rates used in simulations, due to computational constraints, often exceed experimental ones, potentially leading to discrepancies [60].

Looking forward, however, the landscape of MD research on CNMs offers promising avenues [61]. One of the significant improvements in recent years has been the pursuit of enhanced force fields. Continuous research in this domain aims to refine these force fields specifically for carbon nanomaterials, thereby enhancing the accuracy of predictions. Moreover, the emergence of multiscale modelling as a robust approach holds considerable promise. By linking/coupling MD with other simulation methodologies, such as electronic, mesoscopic and/or continuum models, researchers aim to bridge the spatiotemporal gaps between scales. Yet, perhaps one of the most transformative shifts is the integration of data-driven approaches into MD simulations. The infusion of machine learning and artificial intelligence is not merely augmenting computational efficiency but is reshaping the paradigms of simulation. These tools offer optimized parameter selections, predictive capabilities, and the prospect of devising new force fields. Lastly, efforts between experimentalists and computational researchers are fostering iterative refinements in simulation methodologies. This synergy is guiding MD studies closer to experimental observations, ensuring a more harmonized understanding of CNMs.

2.3 Continuum micromechanics

At the next level within the multiscale materials modelling framework, continuum models are a powerful tool for predicting the properties of nanocomposites. These models consider the microstructure of the nanocomposite, including the size, shape, and distribution of the nanoparticles, to predict the macroscopic-homogenized properties of the material. Although this review is focused in micromechanics, continuum models can be used to predict different types of properties (mechanical, thermal, electrical, acoustic, other physical properties…).

There are basically three types of continuum models: analytical, semi-analytical and numerical. The most common analytic models used for nanocomposites are a) Mori-Tanaka's mean field approach, which calculate the properties of the composite by averaging the properties of the nanoparticles and the matrix, weighted by their respective volume fractions; b) Self-consistent models (SCM), where each nanoparticle in the nanocomposite is embedded in a matrix that has the same properties as the nanocomposite itself (this leads to a system of coupled equations that must be solved numerically); and c) Eshelby models, which is more general that the formers and can be used to treat a variety of different nanoparticle geometries and distributions. There are hundreds of works in the literature applying these models to

determine both nanocomposite and also standard fibre-based composites properties. In this sense, interesting references comparing/reviewing all these methods are the article of Y. Wang and Z. Huang [62], the chapter of Yehia A. Bahei-El-Din about Averaging Models of Fibrous Composites in [63], and the recent publication of A. Elmasry, W. Azoti, S. El-Safty and A. Elmarakbi that presents a review comparing different models for effective properties calculation of nano- and micro-composites [64]. Works focused on mechanical properties include: i) nanocomposites' stiffness prediction (i.e. response in the elastic range), as the research done by M.M. Shokrieh, M. Esmkhani, Z. Shokrieh and Z. Zhao for an epoxy resin modified with graphene nanoplatelets [65], the work presented by A. Chiminelli and M. Laspalas for an epoxy resin modified with MWCNTs [66], the work of A. Singh and D. Kumar studying the influence of the functionalization of graphene nanoplatelets in the elastic properties of a modified polyethylene [67] or a more recent work of D. Shin, I. Jeon and S. Yang for graphene modified PET [68]; ii) non-linear behaviour and strength predictions of CNMs, as the approach proposed by J. Nafar Dastgerdi, G. Marquis and M. Salimi introducing interfacial damage/debonding processes in CNTs reinforced polymers [69] or the model developed by W. Azoti and A. Elmarakbi applied to a graphene platelets GPL-reinforced polymer PA6 composite (Generalized Mori-Tanaka) [70]. Other works/studies can be found about the utilization of this type of analytic approaches to develop more advanced models introducing viscoelasticity [71] or creep effects [72], among others. Overall, good correlations with experimental results are obtained for the elastics properties especially at low nanoparticles concentrations, while at higher concentration more significant deviations are usually observed. This is generally explained due to interactions between the nanoparticles at high contents that produce non-homogeneous dispersions and agglomerations. For predictions in the non-linear regime and in terms of strength, it is generally seen that the results are strongly dependent on the particle/polymer interface representation and on the aspect ratios of the particles. Obviously, the issues mentioned at high concentrations are also present in these cases. Apart from this, these models are valuable to evaluate different functionalization of carbon-based nanoparticles.

In addition to the models mentioned above, some semi-empirical analytical models are also well-known for composites, starting with the classical rule of mixture, evolving to Chamis' model and the Halpin–Tsai's model (as a simplified version of the SCM), and leading to more advanced models introducing (again) elasto-plasticity (approaches to yield stress and linearization methods [62]). The Halpin–Tsai approach for aligned reinforcement has been employed widely for the analysis of graphene-based nanocomposites [73]. In this sense, works as the ones developed by Weon et al. [74], Chong et al. [75] and Zarasvand and Golestanian [76] can be highlighted. In the last, the nonlinear tensile stress-strain behaviour of randomly-distributed graphene nanocomposites have been obtained, presenting a good correlation with experimental results in the whole range of the stress-strain curves. In a work published by M. Yang et al. [77], the Halpin-Tsai model was adapted to quantitatively

characterize the effect of temperature on the yield strength of nanofiller-reinforced polymer-matrix nanocomposites. Compared with the classical ones, the model showed a better agreement with the available experimental data from sub-zero temperature to the full glass transition region. Progressing with elasto-plasticity, several Non-linear Mean Field Methods have been developed from the elastic ones, being the Tangent and Secant approaches the most knowns. Some reference publications implementing these methods are the ones of Doghri [78][79]. An advantage of these models is the straightforward implementation. They also allow to study more complex loading cases than other models, including cyclic loads.

Semi-analytical methods are based on global constitutive equations that are evaluated from the local scale using analytic/explicit relations that link the microscopic and the macroscopic properties. The analytical relations are usually dependent on mean field procedures. The most known is the Transformation fields analysis (TFA). It connects analytical and computational approaches by a computational evaluation of the localisation operators. The main concept is replacing the plastic strain field with piecewise uniform fields to reduce the number of macroscopic internal variables. Thereby, a set of reduced constitutive relations for the heterogeneous material can be established, leading to a computational time reduction compared to full numerical models [64]. Reference works of this type of models are the ones published by Dvorak [80][81]. A more recent work published by I.Al. Khattab and M. Sinapius present an interesting implementation of the TFA model as a user routine integrated into RVE-micro scale model [82]. The results reveal that the TFA is a proper method for solving inelastic deformation and other incremental problems in heterogeneous media with many interacting inhomogeneities on a nanoscale level.

Finally, numerical continuum micromechanics models, such as the finite element method (FEM), are considered also powerful approaches for CNMs modelling. In numerical approaches, an acknowledged constitutive model (elasticity, viscoelasticity, elastoplasticity, viscoplasticity…) is assumed in a Representative Volume Element (RVE) to induce an explicit macroscopic model. On one hand, these models allow to introduce more accurate description of the materials nano-morphology [83]. This is one of the limitations of analytic models, that usually require an idealization of the nanoreinforcements' shape, representing them as discs, cylinders or spheres. On the other hand, these models allow to introduce complex nonlinear multi-phase material behaviours. The main disadvantages of finite elements are its computational costs, size dependency of the results and limitations in the development of RVEs with high inclusions volume concentrations and aspect ratios.

RVE based models apply to statistically homogeneous materials. They can be used as repeating unit cell (RUC) when the (nano)composite has a periodic microstructure. Sufficient number of randomly distributed fibers or particles to be contained in the RVE is needed so that the microstructure of a composite could be reflected precisely [62]. This is also linked with the size of the volume studied. Various works reflect the importance of defining a proper RVE size [84]. In this sense, it happens that a larger RVE size gave better prediction accuracy but

resulted in lower computational efficiency. Finally, the boundary conditions are a critical aspect in RUC models, and they have to be defined carefully to represent properly the effect of the reinforcements/particles distribution patterns and the loads applied.

Some first reference publications that can be found about RVE and FEM to estimate properties of polymer nanocomposites are the works of Liu and Chen [85][86]. Particularly, they studied the elastic properties of CNT-reinforced polymers. Chwał and Muc [87][88] applied a similar approach with various boundary conditions to calculate the mechanical properties of SWCNT-polymer nanocomposite. More recent works present a combination of this type of FE continuum models with MD, in similar way to the multi-scale framework presented in this report. For example, recently Barakat et al. published an article where the distribution of mechanical properties of graphene-based polymer nanocomposites is computed using a micro-meso up to macro hierarchical computational approach employing non-equilibrium atomistic MD simulations and continuum FE models [89]. In the same line, the work published by Muhammad et al. can be highlighted [52], where not only mechanical but thermal properties are predicted for graphene-reinforced epoxies. For SWCNT-polymer nanocomposites, Malague et al. proposed a procedure to assess size effects using the atomistic simulations and equivalent continuum model with a large number of CNTs [90].

Elastic RVE/RUC models can be extended to nonlinear cases, providing that the nonlinear constitutive laws for the constituents are available. For example, based on a three-dimensional RVE model, Yuan and Lu [91] conducted a numerical investigation on the elastoplastic behavior of carbon nanotubes (CNTs) reinforced polymer composites. A. Zarasvand et al. [92] also conducted experimental, numerical, and micromechanical studies to determine the nonlinear behavior of CNT-reinforced polymer. When non-linear constitute behaviours are considered, FEM approaches become computationally consuming. To address this limitation, several numerical strategies with reduced computational effort have been developed. Examples are the Voronoi Cell Finite Element Method (VCFEM) [93] [94], the Generalized Method of Cells (GMC) [95], and the Finite Volume Direct Averaging Micromechanics (FVDAM) [96][97][98].

2.4 CNM devices - Graphene Field Effect Transistors

When we arrive to discuss CNM devices that can be considered matures enough to be used in sensing systems, one of the most used configurations is based upon graphene field effect transistors (G-FET). High frequency applications have been in a first time a major goal for this class of devices, and a series of interesting results reporting the fabrication of research level devices working in the GHz domain were published in the 2010's years [100][101][102][103]. Anyway, the problems that were been initially addressed for the graphene transistors to replace silicon MOSFET as the choice alternative for commercial high-performance logic and

high frequency electronics [104], prevented until now their large-scale adoption for this class of applications.

As a follow up, the intense research work realized during these years has produced many interesting results, experimental ad theoretical as well, that have permitted a good insight into the physic mechanism of the GFET structures, paving the way to the definition of an application playground in the biosensing domain, avoiding the HF requirements of a G-FET based ASIC project. A nice summary of the present state of this approach can be found in the recently published review paper of S. Szunerits [105]. It may be foreseen that the use of GFET circuitry will soon find commercial application in wearable flexible sensing systems [106] and in Point-Of-Care systems [107][108]. Advanced experimental results in this field have been recently presented for applications of major interest, like, for example, cancer monitoring [109], COVID-19 screening [110] or glucose monitoring in diabetic patients [111].

Modelling and simulation of GFET device and circuits, in a variety of configurations has certainly given an important contribute to the actual advanced state of the art for design and fabrication. Regarding the electrical properties, a model to calculate the DC characteristics of large-area graphene field-effect transistors was presented initially by Thiele and Schwierz [112]. This paper opened the door to the heuristic approach of correlating the experimental results with the specific characteristics of the graphene material, like the sheet carrier density and transport properties.

As a general description, a G-FET has a structure that can be thought similar to similar to a thin film transistor (TFT), where the 2D graphene layer is used for channel forming. The traditional approach for the electrical simulation of semiconductor FET devices is based on the drift-diffusion model, including the Poisson equation [113]. A Verilog compact model suitable for circuit level design model based of the drift and diffusion scheme has been presented and made freely available by Landauer [114]. The main problem for the direct application of this model to the G-FET structure is the definition of the charge mobility value, that in a 2D material can be largely affected by the presence of impurities, lattice defects and substrate quality. A nice approach to this problem was recently described by Nastasi [115]. They describe extensively the physical and numerical model, including the model for the mobility and its dependence on the applied electric field, and the results obtained on a top gate configuration described by a 2D geometry.

Targeting the sensing of biomolecules (such as proteins and nucleic acids) in biological fluids, co-planar and liquid-immersed-gate configurations are largely preferred in biological G-FET design. This configuration overcomes the standard top-gate or bottom-gate inherited by the flat panel semiconductor industry and presents a new challenge for modelling and simulation approach. The main results of this activity have the production of G-FET models suitable to be used in a circuit simulator, to support the fabrication of complete G-FET based circuit for biosensing applications. Within this context, Jmai [116] presented a model freely distributed in its MATLAB and Verilog implementation, allowing the user to select an appropriate topology

for a system-level design suitable to be used in real life applications. From a higher-level approach, Fuene-Zapico has adapted the Sentaurus Commercial TCAD suite for the simulation of a liquid gate graphene field effect transistor, GFET, used as antibody-based biosensor.

As a bottom line, it must be outlined that The Graphene Flagship's 2D Experimental Pilot Line (2D-EPL), offers prototyping services to academics, SMEs and companies which can benefit from the progresses of Graphene Related Materials (GRM) integration with silicon. The 2D-EPL provide in a multi-project wafer run (MPW) for G-FET circuit including a top/bottom contact with an optional local or global back and liquid gate. Directed to Bio/Gas/Chemical sensors this MPW include a stand-alone G-FET circuit as well as a fully CMOS integration.

In our group in Lisbon, we have simulated and designed a G-FET circuit layout for biosensing that has been fabricated by 2D-EPL. We didn't publish our results yet, as the measurements are not complete, and because we are considering applying for a patent.

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