FLAG-ERA JTC 2017

GRANSPORT

Correlations and defects in graphene and related materials: Charge and heat transport

Mikhail Titov

FLAG-ERA JTC 2017 Project Kick-off Seminar - Graphene -
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Participants

Nijmegen, Karlsruhe, Grenoble, Uppsala, Berlin

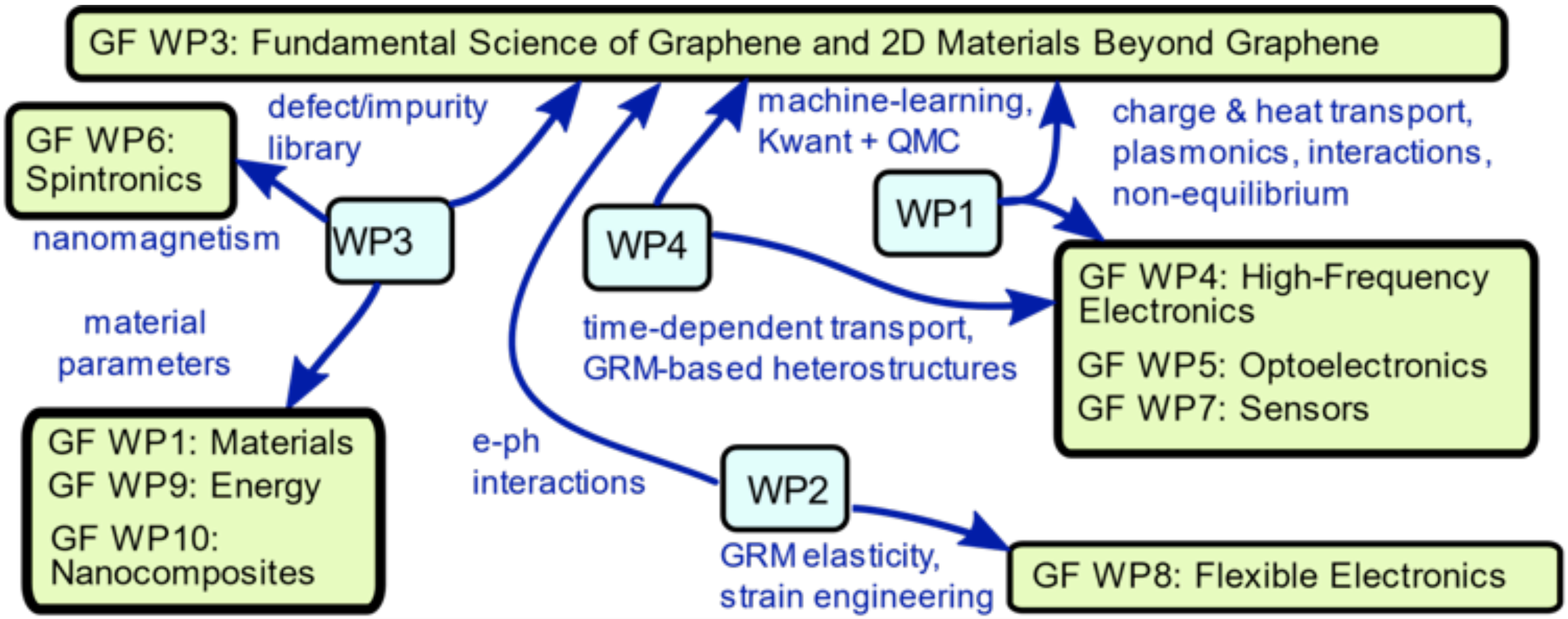
Partner Number	Country	Institution/ Department	Principal Investigator (PI)	Co-Investigators	Other participants
1 *Coordinator*	Netherlands	Radboud University Nijmegen (**RU**) / IMM	**M. Katsnelson**	M. Titov A. Akhmerov (Delft)	S. Wiedmann M. Wimmer A. Rudenko post-doc
2	Germany	Karlsruhe Institute of Technology (**KIT**)/ INT	**I. Gornyi**	A. Mirlin B. Narozhny	R. Danneau R. Krupke PhD student
3	France	**CEA** Grenoble / INAC-PHELIQS	**X. Waintal**	C. Groth	PhD student
4	Sweden	Uppsala University (**UU**) / Physics & Astronomy	**O. Eriksson**	J. Nilsson B. Sanyal	PhD student
5 *not requesting funding*	Germany	Free University Berlin (**FUB**) / Department of Physics	**K. Bolotin**		PhD student (funded externally)

combines theory and experiment

Duration: 36 Months

Starting: April 1, 2018

Synergy with Graphene Flagship



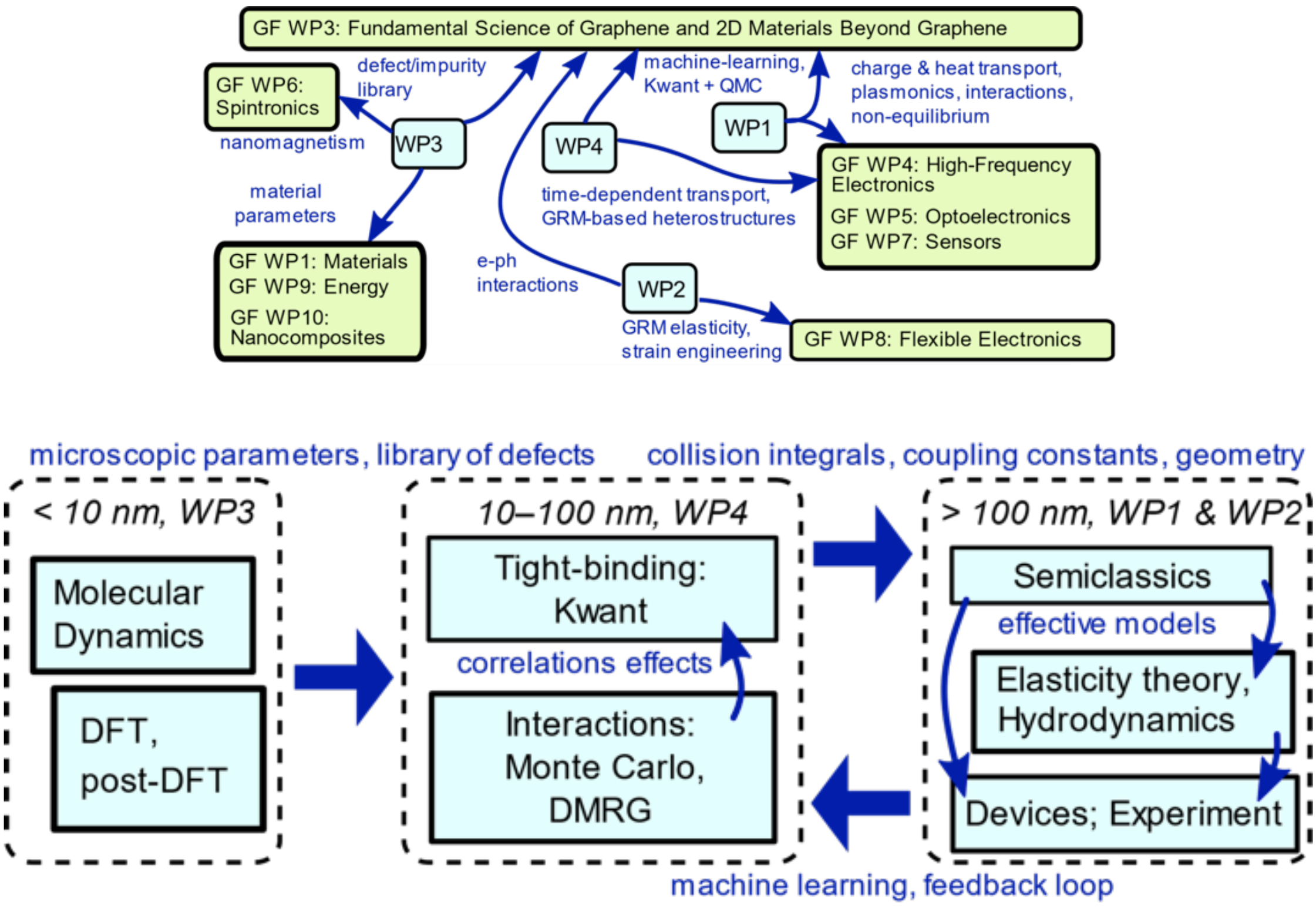
WP1: Transport, correlations, and non-equilibrium kinetics

WP2: Elasticity of 2D membranes and its influence on transport properties

WP3: Novel *ab initio* methods for 2D materials

WP4: Multiscale modelling of GRM and GRM heterostructures

Up-scaling of simulations



WP 1	**Transport, correlations, and non-equilibrium kinetics**	Start: M1	End: M36

Contribution of project partners (WP Leader: P1 – RU Nijmegen)

Partner number		**1 Nijmegen**	2 Karlsruhe	3 Grenoble	4 Uppsala	5 Berlin		
Person*months, senior+hired		4+36	4+0	4+0	2+0	4		

WP1 deals with **transport, kinetics, and interactions** in GRM and hybrid structures. The effective models, which are developed within the WP1, crucially employ the input from the **multiscale numerical simulations** (WP3 and WP4) and from analytic theories. The WP1 considers fundamental aspects of disordered graphene and GRM and addresses such issues as correlation effects, far-from-equilibrium kinetics and plasmonics, kinetic-equation and hydrodynamics, physics of Moiré structures, superconducting hybrid systems, proximity effects, charge and heat transport, and excitonic effects.

Tasks

T1.1 **Charge and heat transport in disordered graphene and GRM** **(M1-M27: Responsible: P2; Involved: P1, P3, P5)**

ST1.1.1. Developing numerical tools for simulating nonlinear hydrodynamics in GRM in the presence of defects, macroscopic inhomogeneities, recombination, excitonic correlations, nanostructuring, and arbitrary boundary conditions.

ST1.1.2. Developing analytical theory of viscous charge and heat magnetotransport and non-local response in functionalized graphene and GRM.

T1.2 **Noise, far-from-equilibrium kinetics and plasmonics in graphene and GRM** **(M7-M18: Responsible: P1; Involved: P2, P3)**

ST1.2.1. Developing large-scale kinetic-equation framework far from equilibrium.

ST1.2.2. Employing numerical techniques (e.g., DMRG) developed for strongly correlated 1D systems to kinetics and emergent transient behaviour in GRM with strong interactions.

ST1.2.3. Experimental study of transport noise and non-equilibrium phenomena in GRM.

T1.3 **Functionalized graphene-based systems** **(M1-M36: Responsible: P2; Involved: P1, P3, P4)**

ST1.3.1. Modelling gate-controlled superconducting proximity effects in bilayer graphene and GRM using **Kwant** and its extensions (WP4).

ST1.3.2. Modelling and experimental study of GRM decorated by resonant rare-earth impurities.

T1.4 **Layered GRM-based structures** **(M13-M36: Responsible: P1; Involved: P2, P3, P4, P5)**

ST1.4.1. Excitonic effects in graphene double-layers and in GRM-based heterostructures.

ST1.4.2. Designing and experimentally exploring virtual topological materials based on GRM heterostructures functionalized with materials with strong spin-orbit interaction.

Deliverable	Month	Title of deliverable
D1.1	12	Analytical theory of viscous heat and charge (magneto) transport
D1.2	18	Experimental validation of the kinetic and hydrodynamic frameworks for out of equilibrium transport and noise in GRM
D1.3	24	Report on modelling and experimental studies on functionalized graphene and GRM
D1.4	32	Modelling and observation of excitonic effects and instabilities in GRM-based heterostructures and graphene double layers
D1.5	36	Realization of topological materials based on functionalized GRM heterostructures

WP 2	**Elasticity of 2D membranes and its influence on transport properties**	Start: M 1	End: M 36

Contribution of project partners (WP Leader: P2 – KIT Karlsruhe)

Partner number		1 Nijmegen	**2 Karlsruhe**	3 Grenoble	4 Uppsala	5 Berlin		
Person*months, senior+hired		4+0	4+36	0	0	8		

WP2 is devoted to the **theoretical and experimental study of elasticity** of 2D membranes and its influence on **transport properties** of GRM, both suspended and on the substrate. Our main goal is to explore the renormalization of mechanical constants of 2D materials caused by their out-of-plane crumpling in strain-engineered membranes. The activities of WP2 cover such topics as dynamical elasticity under **external driving**, attenuation of flexural modes, the Poisson ratio in disordered membranes, the detachment transition for membranes on substrates, the thermodynamics of Moiré and striped phases, the effect of strong electron correlations on elastic properties, and electronic transport in engineered structures using the combination of analytical tools and Monte-Carlo simulations. WP2 will provide input for studying charge and heat transport in WP1.

Tasks

T2.1 **Elasticity of suspended membranes** **(M1-M18: Responsible: P5; Involved: P1, P2)**

ST2.1.1. Poisson ratio in disordered membranes of graphene and GRM: Theory
ST2.1.2. Poisson ratio in 2D membranes: Experiment
ST2.1.3. Dynamical elasticity under external driving and the attenuation of flexural modes

T2.2 **Thermodynamics of membranes on substrates** **(M7-M27: Responsible: P1; Involved: P2, P5)**

ST2.2.1. Thermal expansion coefficient of GRM on substrate and of heterostructures of GRM
ST2.2.2. “Bubbles” and detachment transition for graphene on substrates
ST2.2.3. Interplay of elasticity and Moiré patterning in van der Waals heterostructures

T2.3 **Effect of electron correlations on elastic properties of 2D membranes** **(M13-M36: Responsible: P2; Involved: P1, P5)**

ST2.3.1. Effect of electron correlations on elastic properties of disordered and engineered 2D membranes (monolayer graphene, bilayer graphene, GRM).
ST2.3.2. Developing theory of buckling transition under stress in 2D membranes with electron correlations.

T2.4 **Role of elasticity in electron transport** **(M1-M36: Responsible: P2; Involved: P1, P5)**

ST2.4.1. Experimental investigation of charge and heat transport in controllably strained graphene and in monolayer transition-metal-dichalcogenides.
ST2.4.2. Developing theory of charge and heat transport in strained graphene and GRM.
ST2.4.3. Relaxation and thermoelectric phenomena caused by electron-phonon scattering in graphene with resonant impurities.

Deliverable	Month	Title of deliverable
D2.1	12	Experimental validation of the theory of the Poisson ratio
D2.2	18	Report on the theory of thermodynamics of membranes on substrates
D2.3	24	Theory of buckling transition under stress in GRM membranes
D2.4	36	Experimental observation of thermoelectric phenomena in strain-engineered GRM and graphene

WP 3	**Novel *ab initio* methods for 2D materials**	Start: M 1	End: M 36

Contribution of project partners (WP Leader: P4 – UU Uppsala)

Partner number		1 Nijmegen	2 Karlsruhe	3 Grenoble	**4 Uppsala**	5 Berlin		
Person*months, senior+hired)		4+0	2+0	4+0	4+36	0		

WP3 develops ab initio modelling to extract effective tight-binding (TB) parameters that can be used to **model large-scale devices.** The results will be stored in a file format tailored for reading by TB solvers such as Kwant. WP3 will focus on ab initio modelling of various pristine GRMs, modelling spin-orbit interaction, DFT band structure computation, construction of effective TB Hamiltonians, modelling of Anderson impurities in GRM, ab initio studies of grain boundaries, modelling van-der-Waals heterostructures, modelling optical properties of graphene and GRM in the presence of defects, and description of excitonic features in optical spectra identifying unique signatures of specific defects. WP3 will provide microscopic inputs and *ab initio* calculations for WP1 and WP4.

Tasks

T3.1 **Ab initio modelling of pristine GRMs (M1-M24; Responsible: P4; Involved: P1, P3)**

ST3.1.1. Developing novel computational tools for benchmarking, verification, and upscaling DFT-based calculations

ST3.1.2. Providing input parameters and benchmarks for model tight-binding Hamiltonians. Establishing boundary conditions and input parameters (effective masses, interface potentials, excitonic offsets, viscosity) for kinetic and hydrodynamic equations.

T3.2 **Impurities in graphene and GRM (M1-M27; Responsible: P4; Involved: P1, P3)**

ST3.2.1: Characterisation of defects in 2D materials from ab initio theory. Extraction of tight-binding parameters for defected 2D materials using DFT and maximally localised Wannier functions. Getting scattering potential from ab initio calculation to feed an effective tight-binding model. This will be used as an input for Kwant transport calculations (WP4).

ST3.2.2: Establishing **"the Library" of defects** and impurities in graphene and GRM.

ST3.2.3: Post-DFT modelling of nano-magnetism (exchange interactions, spin-orbit effects, spin-torque) in 2D materials in the presence of magnetic adatoms, clusters and molecules and of van der Waals heterostructures (e.g., graphene/WSe_2)

T3.3 **Ab initio studies of grain boundaries and interlayer binding in layered structures (M7-M36; Responsible: P4; Involved: P3)**

ST3.3.1: Predicting the electronic, transport, and optical properties of heterostructures using an *ad hoc* scheme. Developing a **machine-learned approach** to improve the ad hoc scheme based on actual ab initio calculations (DFT and possibly beyond) of various heterostructures.

ST3.3.2: Employing and testing the post-DFT methodology on van der Waals heterostructures: bilayer graphene, functionalised graphene, graphene on hBN.

T3.4 **Optical properties of GRM in the presence of defects (M13-M36; Responsible: P4; Involved: P1, P2, P3)**

ST3.4.1: X-ray absorption spectroscopic studies for capturing signatures of specific defects in 2D materials, excitonic features in optical absorption spectra in presence of defects.

ST3.4.2: Combining materials with different electronic properties (metallic, insulating, and possibly with different band alignments) in order to obtain promising perspective optoelectronic devices.

Deliverable	Month	Title of deliverable
D3.1	12	Database with TB parameters for many GRMs (also continued updates)
D3.2	12	Defect library (also continued updates)
D3.3	24	Properties of functionalized GRMs
D3.4	36	Defect-related spectroscopic signatures

WP 4	**Multiscale modelling of GRM and GRM heterostructures**	Start: M 1	End: M 36

Contribution of project partners (WP Leader: P3 – CEA Grenoble)

Partner number	1 Nijmegen	2 Karlsruhe	**3 Grenoble**	4 Uppsala	5 Berlin
Person*months, senior+hired	4+0	4+0	4+36	2+0	0

WP4 is focused on multiscale and multiphysics modelling, the innovative and unique concept of GRANSPORT. The WP4 will develop the necessary bridges needed to interconnect the different approaches of GRANSPORT. The WP4 will provide both formalism and software to enable multi-scale modelling of graphene and GRM using an integrated combination of such tools as the theory platform, Kwant code, and real-time quantum Monte-Carlo techniques.

Tasks

T4.1 **Integrating the ab initio input into the tight-binding approach** **(M1-M18: Responsible: P3; Involved: P1, P2, P4)**

ST4.1.1. Developing a suitable abstraction model for interfacing the three different simulation levels (ab-initio, tight-binding and semi-classical). Coordination with T3.1 and T3.2 for engaging best-optimised transport codes with ***ab initio*/tight-binding model elaboration** for exploring charge and spin transport in disordered GRM and van der Waals solids.

ST4.1.2. Enhancing Kwant such that systems with defects/impurities can be constructed using the Impurity Library (T3.2) for simulating realistic mesoscale devices. Testing localisation transitions in systems with adatoms and vacancies.

T4.2 **Integrating the real-time quantum Monte-Carlo techniques into Kwant** **(M7-M27: Responsible: P3; Involved: P1, P2)**

ST3.2.1: Developing high order diagrammatic Monte-Carlo technique for treating electron-electron interactions within the Kwant code.

ST3.2.2: Application to clean and disordered GRM devices. Study of electron-electron interaction induced renormalization of single electron properties.

T4.3 **Collision integrals from Kwant** **(M13-M30: Responsible: P3; Involved: P1, P2, P4)**

ST4.3.1. Elaborating the formalism and software to obtain the elastic collision integrals for the semi-classical kinetic approach from the Kwant code.

ST4.3.2: Developing the methodology for calculating the inelastic collision integrals for the semi-classical approach using the technique developed in T4.2

T4.4 **Real-time transport (machine-learning assisted) at the quantum or semi-classical level** **(M10-M36: Responsible: P1; Involved: P2, P3)**

ST4.4.1: Developing a Markov chain Monte-Carlo prototype for solving semiclassical transport equations in the time domain. Exploration of various machine learning strategies to model the semi-classical behaviour.

ST4.4.2 Developing an “advanced prototype”-level code for time-resolved quantum transport in GRM devices.

Deliverable	Month	Title of deliverable
D4.1	15	Interfacing the three simulation levels
D4.2	18	Demonstration of high order many-body perturbation theory calculations on GRM device
D4.3	24	Extracting collision integral data from Kwant
D4.4	36	Demonstration of time dependent simulation of a GRM device

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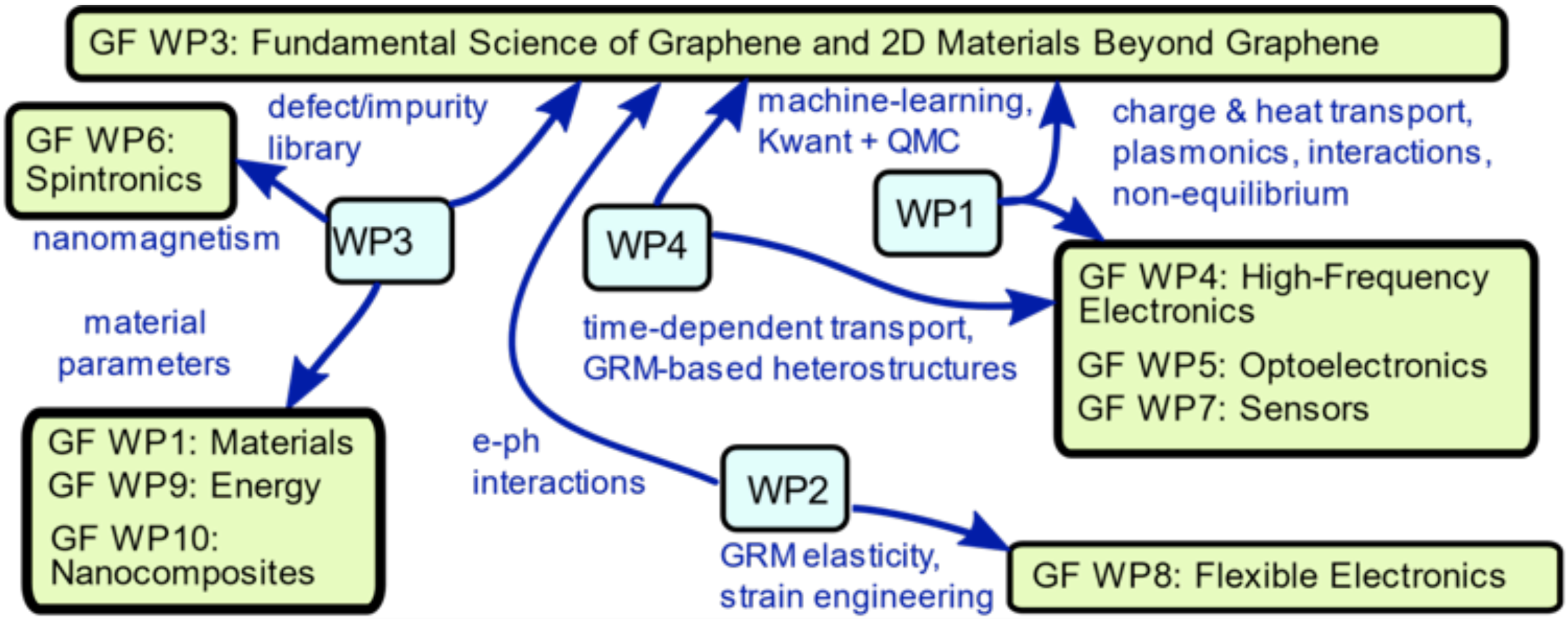

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Thank you very much for your attention