Banff International Research Station
for Mathematical Innovation and Discovery

Coupled Mathematical Models for Physical and Biological Nanoscale Systems and Their Applications

August 28 - September 2, 2016

Organizers: Luis Bonilla (Universidad Carlos III de Madrid, Spain),
Efthimios Kaxiras (Harvard University, United States)
Roderick Melnik (Wilfrid Laurier University, Canada)

PROGRAM AND ABSTRACTS

OBJECTIVES

Due to the vastness, novelty and complexity of the interface between mathematical modelling and nanoscience and nanotechnology, many important areas in these disciplines remain barely explored. In progressing further, multidisciplinary research communities have come to a clear understanding that, along with experimental techniques, mathematical modelling and analysis have become crucial in the study, development, and applications of systems at the nanoscale. This workshop is aimed at bringing together researchers from these communities, experts who are working on different aspects of the analysis, modeling, and applications of nanoscale systems, with particular focus on low dimensional nanostructures and coupled mathematical models for their description. The development of such models requires concerted efforts from mathematicians, physicists (both theoreticians and experimentalists), and computational scientists, including those working on biological nanostructures.

By bringing together the researchers from these three communities, the main objective of the workshop is to
(a) summarize the state-of-the-art coupled mathematical models, their analysis, and computational techniques, as it then exist, for modeling low dimensional nanostructures,
(b) identify critical problems of major importance that require solution and prioritize them,
(c) analyze feasibility of existing mathematical and computational methodologies for the solution of some such problems, and their analysis, and
(d) use some of the workshop working sessions to explore promising approaches in addressing identified challenges.

Impact and implications of this workshop are expected to be far reaching on several new inroads of this interdisciplinary field, where we will put our main efforts. Some of these include, but not limited to
a) the analysis of coupled effects in spin polarization,
b) spatio-temporal properties of nanoscale systems, accounting for coupled effects,
c) coupled application-driven mathematical models, topological structures, and open problems.

We will have four main plenary talks that will give state-of-the-art overviews of the subject area from perspectives of applied mathematics, physics, and computational science communities, as well as from a point of view of experimentalists. These talks should help identify the areas where joint efforts should be directed to, and they will set up the scene for further work. The workshop features many senior distingushed participants who will present their current research and, when necessary, a specific time will be allocated for on-site demonstrations of software and explanations of experimental tools applied in the analysis of physical and biological nanostructures. We made extra efforts to attract young talented researchers working in this interdisciplinary field and ensured appropriate representation of women. Several young researchers who are currently working with our senior invitees will also have the opportunity to present their works at this workshop.

Among many areas, advances in the development of coupled mathematical models and their analysis for physical and biological nanoscale systems impact applications in biotechnology and medicine, quantum information processing and optoelectronics. The main topic of this workshop offers exciting new challenges that are intrinsically interdisciplinary and should be addressed by a multidisciplinary team and the BIRS environment is an ideal place for its meeting.

MEETING FACILITIES

The meeting will take place in the new TransCanada Pipelines Pavilion (TCPL) at the Banff International Research Station (BIRS).

Open wireless Internet access("wifi", no password required) is available is available in all areas of BIRS, including the TCPL building. Please consult the Technology page for more detail on equipment.

The BIRS is physically located on the campus of The Banff Centre. BIRS occupies Corbett Hall and the TransCanada Pipelines Pavilion. TransCanada Pipelines Pavilion is wheelchair accessible, and Corbett Hall is wheelchair accessible through Max Bell. A detailed desription of these facilities can be found here.

TCPL 201 is our main lecture room. It features a tiered lecture auditorium, has chalkboards, an LCD projector and screen, and a document camera. We will use other breakout rooms for brainstrorming sessions and discussions located in the TCPL building.

Maps are provided on the next page and further details on the meeting facilities can be found here.

Participants of BIRS programs are housed in Corbett Hall at the Banff Centre. Our workshop participants are expected to arrive on August 28, Sunday afternoon or evening (check-in is after 4 p.m.) and to depart on September 2, Friday midday (check-out is at noon). Accommodation and meals are provided for all invitees of this workshop (the organizers and participants) for this period.

Check-in desk at the Banff Centre is located in the Professional Development Centre (PDC). The desk is open 24 hours* so participants can check in anytime. Here you will be given the key to your room in Corbett Hall as well as any information useful for BIRS participants. During your stay at BIRS, you can be contacted by telephone through The Banff Centre switchboard, which is open 24 hours, at +1-403-762-6100.

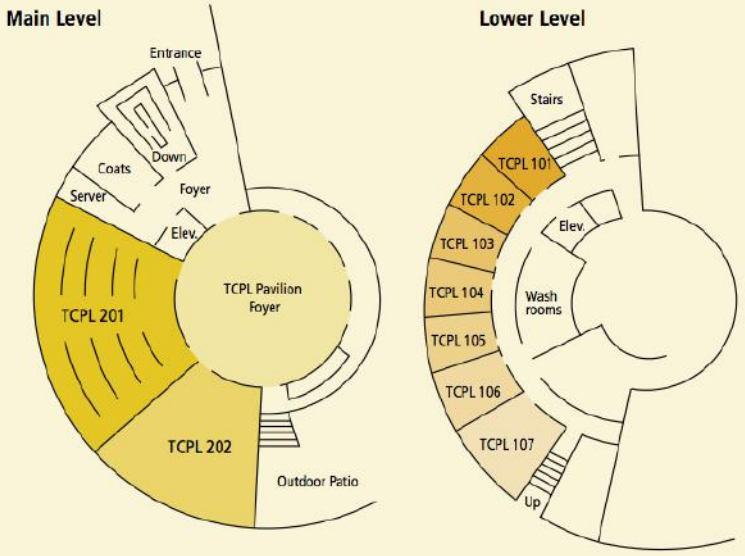
Registration should be straight-forward as the Banff Centre should be expecting your arrival. They will ask you for a Credit Card imprint. This is only to cover your incidental expenses, and to allow you to use the telephone in your bedroom. Without it your phone will not work.

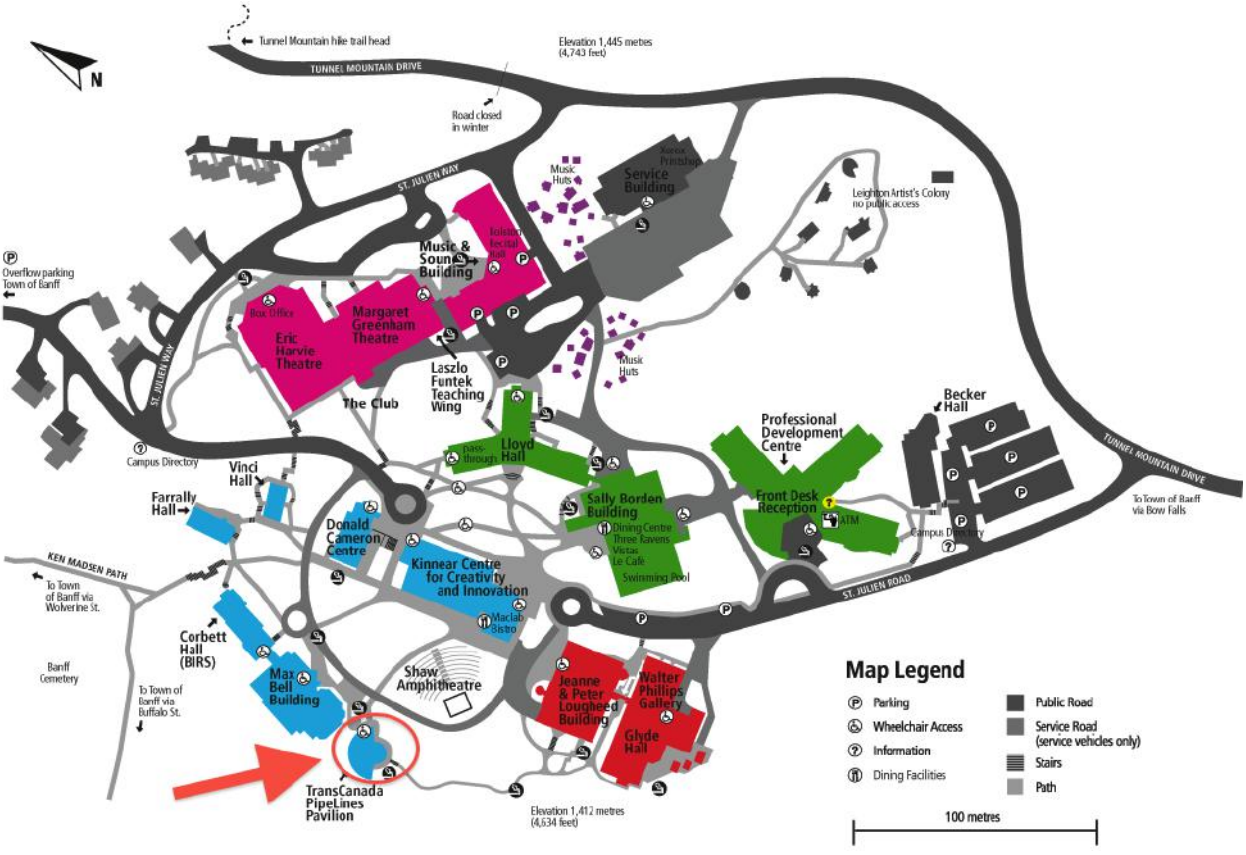
After you have registered and received your key, please proceed to Corbett Hall. Corbett Hall is the home of BIRS and there you will be able to find more information about the many facilities available to you at the Banff Centre. Every bedroom at BIRS has a telephone and has an ethernet network port for fast connectivity to the Internet. Wireless is also available.

Further information on accommodations can be found here.

TransCanada PipeLines Pavilion

A sensitively designed structure of wood, glass, and Rundle rock, the TransCanada PipeLines Pavilion features magnificent views of the Vermilion Lakes and the Bourgeau mountain range. The Pavilion houses ten fully-equipped meeting rooms and a central reception area.





BIRS LOCATION AND GENERAL INFORMATION

BIRS is located at the Banff Centre in Banff, Alberta, Canada. For more information about The Banff Centre, including its arts programmes and recreation facilities, please visit: www.banffcentre.ca .

Most participants will be arriving and departing from the Calgary International Airport. There is shuttle service from the Airport to the Banff Centre (Professional Development Centre). Reservations are recommended (and are necessary for the trip returning to the airport). The Banff Airporter Shuttle offers a 15% discount to all BIRS participants. To get the discount, enter the promo code "birs" at the payment screen. Reserve online at: http://www.banffairporter.com/ Tel: 1-888-HIWAY-01 (1-888-449-2901) in the US and Canada.

If you are renting a car then you should be aware that in order to enter Banff National Park (in which BIRS is located) you need to pay a daily user fee. For more on this you may go to the Parks Canada website:
http://www2.parkscanada.gc.ca/pn-np/ab/banff/visit/tarifs-fees_e.asp?park=1

You will pay this as you enter into the National Park. The Banff Centre will provide free parking for you for your stay at BIRS.

One aternoon at the workshop is free for exploring the Banff region,
the spectacular scenery of the mountains surrounding it, and the many
wonderful outdoor activities it offers.

The following are some tourism websites:

- Banff/Lake Louise Tourism Bureau
- Discover Banff

There is a useful map showing the location of the Banff Centre and some of the main hotels, restaurants, and attractions of Banff at:http://www.discoverbanff.com/Maps

PARTICIPANTS

The list of participants can be found at the BIRS website of the workshop by clicking here.

TALKS AND DISCUSSIONS

Plenary talks will be up to a max of 40 mins with 5 mins questions, regular talks will be around 15 mins with 5 mins questions. There will be additional time for discussions in the afternoon. Topics for the study groups will be announced and sign-up sheets posted onsite.

You can submit further your comments on the topics of the workshop to any of the organizers (and, of course, open problems are still very welcome and needed!). Also, we would like to encourage the submission of your presentations to be available online. Finally, we would like to encourage you to submit your preprints and reprints relevant to this workshop (not necessarily on the topic of your main presentation at Banff, but of relevance to the topics of this workshop). It will help to share the information between the participants of this workshop as well as networking. The site for all these submissions will be provided (you should be able to do that before, during, and after the workshop). Wirelesss access will be available throughout the Banff International Research Station).

PROCEEDINGS

All participants are encouraged to submit their work for publication in a proceedings. Original (research and review) articles will be published by Springer as a separate book. Manuscripts should be emailed to the organizers and will be peer-reviewed. Please submit your manuscript as soon as possible after the meeting. The final deadline for submission will be November 15, 2016. There is no page limit.

Guidelines for manuscript preparation will be communicated to all participants who confirmed their intention to submit.

SCHEDULE

MEALS

*Breakfast: 7:00 – 8:45 am, Vistas Dining Room, Monday – Friday
*Lunch: 12:00 am – 13:00 pm, Vistas Dining Room, Monday – Friday
*Dinner: 18:00 – 19:30 pm, Vistas Dining Room, Sunday – Thursday

Coffee Breaks: As per daily schedule, TCPL Foyer

MEETING ROOMS

All lectures will be held in the TransCanada Pipelines Pavillion (TCPL). The main lecture room for our workshop is TCPL 201. An LCD projector and screen, and a document camera are available in that room. Our study group brainstorming sessions and discussions are also located in the TCPL building. Please respect that all other space has been contracted to other Banff Centre guests.

Coupled Mathematical Models for Physical and Biological Nanoscale Systems and Their Applications

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Sunday, Aug 28

16:00	17:30	Check-in begins at 16:00 on Sunday and is open 24 hours (Front Desk - Professional Development Centre)
18:00	19:30	Dinner (Vistas Dining Room)
20:00	22:00	Informal gathering (Corbett Hall Lounge (CH 2110))

Monday, Aug 29

07:00	08:45	Breakfast (Vistas Dining Room)
08:45	09:00	Introduction and Welcome by BIRS Station Manager (TCPL 201)
09:00	09:45	Plenary 1 (Sachrajda) (TCPL 201)
09:45	10:45	Talks 1 (Birnir, Neu, Rubi) (TCPL 201)
10:45	11:00	Coffee Break (TCPL Foyer)
11:00	12:00	Talks 2 (Di Ventra, Krishnamurthy, Prados) (TCPL 201)
12:00	13:00	Lunch (Vistas Dining Room)
13:00	14:00	Guided Tour of The Banff Centre (Corbett Hall Lounge (CH 2110))
14:00	14:30	Group Photo (TCPL Foyer)
14:30	15:15	Study Groups (TCPL 201)
15:15	15:30	Coffee Break (TCPL Foyer)
15:30	16:30	Talks 3 (Ortner, Shirodkar, Cazeaux) (TCPL 201)
16:30	17:30	Discussion (TCPL 201)
18:00	19:30	Dinner (Vistas Dining Room)

Tuesday, Aug 30

07:00	08:45	Breakfast (Vistas Dining Room)
09:00	09:45	Plenary 2 (Nelson) (TCPL 201)
09:45	10:45	Talks 4 (Carpio, Bonilla, Yatsyshin) (TCPL 201)
10:45	11:00	Coffee Break (TCPL Foyer)
11:00	12:00	Talks 5 (Privman, Sanchez, Wang) (TCPL 201)
12:00	13:00	Lunch (Vistas Dining Room)
13:00	13:45	Plenary 3 (Zabaras) (TCPL 201)
13:45	14:55	Study Groups (TCPL 201)
14:55	15:15	Talk 6 (Gusarov) (TCPL 201)
15:15	15:30	Coffee Break (TCPL Foyer)
15:30	16:30	Talks 7 (Grahn, Ruiz-Garcia, Bairamov) (TCPL 201)
16:30	17:30	Discussion (TCPL 201)
18:00	19:30	Dinner (Vistas Dining Room)
19:30	20:15	Posters (Hoiles, Ruiz-Garcia, Carr+Fang, Leipzig Max-Planck Institute poster, ASU group poster) (TCPL 201)

Wednesday, Aug 31

07:00	08:45	Breakfast (Vistas Dining Room)
09:00	09:45	Plenary 4 (Cances) (TCPL 201)
09:45	10:45	Talks 8 (Platero, Willatzen, Prabhakar) (TCPL 201)
10:45	11:00	Coffee Break (TCPL Foyer)
11:00	12:00	Talk 9 (Computational Tools, Methods & Software Overview (Caflisch)) (TCPL 201)
12:00	13:00	Lunch (Vistas Dining Room)
13:30	18:00	Free Afternoon (Banff National Park)
18:00	19:30	Dinner (Vistas Dining Room)

Thursday, Sep 1

07:00	08:45	Breakfast (Vistas Dining Room)
09:00	09:45	Plenary 5 (Tuszynski) (TCPL 201)
09:45	10:45	Talks 10 (Luskin, Massatt, Carr+Fang) (TCPL 201)
10:45	11:00	Coffee Break (TCPL Foyer)
11:00	12:00	Talks 11 (Caflisch, Li, Fan) (TCPL 201)
12:00	13:00	Lunch (Vistas Dining Room)
13:00	14:00	Talks 12 (Plechac, Kaupuzs, Serna) (TCPL 201)
14:00	15:15	Study Groups (TCPL 201)
15:15	15:30	Coffee Break (TCPL Foyer)
15:30	17:30	Last Session with Overall Review (Kaxiras) and Discussion (TCPL 201)
18:00	19:30	Dinner (Vistas Dining Room)

Friday, Sep 2

07:00	08:45	Breakfast (Vistas Dining Room)
09:00	10:30	Outcomes (TCPL 201)
10:30	11:00	Coffee Break (TCPL Foyer)
11:30	12:00	Checkout by Noon (Front Desk - Professional Development Centre)
12:00	13:30	Lunch from 11:30 to 13:30 (Vistas Dining Room)

The 2016 BIRS Workshop on Coupled
Mathematical Models for Physical and
Biological Nanoscale Systems and
Their Applications,
Banff, Alberta, Canada,
August 28 - September 2, 2016

Nonlinear Quantum Mechanics

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We model the dynamics of electrons in doped quantum wells driven by terahertz radiation and a superlattice biased by a dc voltage. We compute coherent, self-consistent electron states, density matrix equations of motion, and dipole absorption spectra. The model simultaneously accounts for intersubband transitions and many nonlinear phenomena that have been observed in these systems. We predict a bistable response for strong terahertz fields and bifurcations to coherent time-periodic quantum states. These bifurcation include, period-doubling bifurcations, producing a subharmonic response, Hopf bifurcations producing an incommensurate frequency response, and a cascade of period doubling bifurcations to a strange attractor. We also see a cascade of quasi-periodic orbits on the Hopf torus to a strange attractor. These bifurcation have been difficult to measure in single quantum wells. Therefore we design super-lattice heterostructures of quantum wells where these bifurcations occur and are easier to measure.

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Tumor induced angiogenesis

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Angiogenesis is a multiscale process by which blood vessels grow from existing ones and carry oxygen to distant organs. Angiogenesis is essential for normal organ growth and wounded tissue repair but it may also be induced by tumors to amplify their own growth. Mathematical and computational models contribute to understanding angiogenesis and developing anti-angiogenic drugs, but most work only involves numerical simulations and analysis has lagged. A recent stochastic model of tumor induced angiogenesis including branching, elongation, and anastomosis (fusion) of blood vessels captures some of its intrinsic multiscale structures, yet allows one to extract a deterministic integropartial differential description of the vessel tip density [1].

Vessel tips proliferate due to branching, elongate following Langevin dynamics and, when they meet other vessels, join them by anastomosis and stop moving. Stalk endothelial cells follow the tip cells, so that the trajectories thereof constitute the advancing blood vessel. Anastomosis keeps the number of vessel tips relatively small, so that we cannot use the law of large numbers to derive equations for their density. Nevertheless, we show that ensemble averages over many replicas of the stochastic process correspond to the solution of the deterministic equations with appropriate boundary conditions [2]. Most of the time, the density of tips sprouting from a primary blood vessel advances chemotactically towards the tumor driven by a soliton similar to the famous Korteweg-de Vries soliton. There are two collective coordinates whose slow dynamics changes the shape and velocity of the soliton. Analyzing the equations for the collective coordinates paves the way for controlling angiogenesis through the soliton, the engine that drives this process [3].

References

[1] L.L. Bonilla, V. Capasso, M. Alvaro, and M. Carretero, *Hybrid modeling of tumor-induced angiogenesis*, Phys. Rev. E **90**, 062716 (2014).

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Compressed Modes fo rMaterial Interface Problems

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Much recent progress in data science (e.g., compressed sensing and matrix completion) has come from the use of sparsity and variational principles. This talk is on transfer of these ideas from information science to differential equations and materials physics. The focus is on variational principles and differential equations whose solutions are spatially sparse; i.e., they have compact support. Analytic results will be presented on the existence of sparse solutions, the size of their support and the completeness of the resulting "compressed modes" (see Refs. [1, 2, 3, 4, 5]). Applications of compressed modes for simulation of interfaces (e.g., phase transitions, surface diffusion and pattern formation) will be described.

References

[1] H. Brezis, *Solutions with compact support of variational inequalities*, Russian Math. Surveys **29**, pp. 103-108 (1974).

[2] H. Brezis and A. Friedman, *Estimates on the support of solutions of parabolic variational inequalities*, Illinois J. Math. **20**, pp. 82-97 (1976).

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Some Mathematical and Numerical Challenges in First-Principle and Multiscale Modeling of Nano-Systems

E. Cancès[1]

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The modeling and simulation of nano-systems gives rise to a formidable list of exciting mathematical and numerical problems of various difficulties. In this talk, I will focus on two problematics:

1. the modeling and simulation of (infinite or very large) aperiodic systems;
2. the computation of error estimators.

The general theory of one-particle linear models for homogeneous aperiodic materials was developed by Bellissard and collaborators in the 1990s, and was very successful in, notably, explaining with mathematical rigor the quantum Hall effect and some of the electronic properties of quasicrystals (see [1] and references therein). Homogeneous multilayer 2D materials, in which aperiodicity originates from incommensurability and/or the presence of defects, can be described within this framework. On the other hand, the theory of self-consistent models (Hartree-Fock, Kohn-Sham, ...) for homogeneous aperiodic solids is not yet completely understood from a mathematical point of view [2]. The main difficulty is due to the long-range nature of the Coulomb interaction, which is only partially screened in insulators and semiconductors. Another important class of aperiodic systems encountered in chemistry and biology consists of solvated molecules. It is not possible to simulate both the solute and each and every solvent molecule surrounding it with brute force first-principle models. I will briefly present a multiscale QM/MM/PCM model [3], developed in the framework of an interdisciplinary collaboration between chemists and mathematicians, which allows one to run molecular dynamics simulations of very large solvated molecules.

The second part of the talk will be concerned with the design of certified and optimized molecular simulation methods. Indeed, simulation packages should return not only the estimated value of the computed property, but also guaranteed error bars allowing one to estimate the accuracy of the simulation. Besides, since molecular simulation consumes about 20% of the CPU time available in scientific computing centers, it is important to try and optimize the use of the computational means, that is to minimize the computational cost to reach the desired accuracy. All this requires effective *a posteriori* error bars. Some preliminary results on the construction of discretization and algorithmic error bars for Kohn-Sham models will be presented [4]. The difficult question of model error will also be briefly addressed.

References

[1] J. Bellissard, *Noncommutative geometry of aperiodic solids*, Geometric and Topological Methods for Quantum Field Theory, (Villa de Leyva, 2001), pp. 86-156, World Sci. Publishing, River Edge, NJ, (2003).

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Biofilm mechanics and patterns

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From multicellular tissues to bacterial colonies, three dimensional cellular structures arise through the interaction of cellular activities and mechanical forces. Simple bacterial communities provide model systems for analyzing such interaction. Biofilms are bacterial aggregates attached to wet surfaces and encased in a self-produced polymeric matrix. Biofilms in flows [1, 2] form filamentary structures that contrast with the wrinkled layers observed on air/solid interfaces [3, 4]. We are able to reproduce both types of shapes through elastic rod and plate models [2, 4] that incorporate information from the biomass production and differentiations process, such as growth rates, growth tensors or inner stresses, as well as constraints imposed by the interaction with environment. A more precise study of biofilm dynamics requires tackling water absorption from its surroundings and fluid transport within the biological system. This process alters the material properties of the biofilm and the overall stresses. We analyze whether poroelastic approaches [5] can provide a suitable combined description of fluid-like and solid-like biofilm behavior.

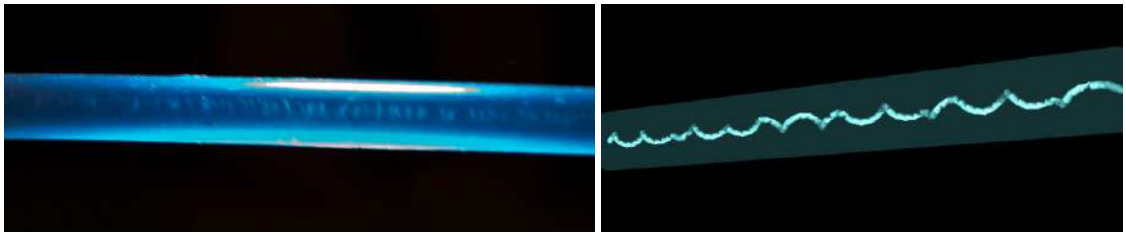

Figure 1: (a) Helical biofilm formed in a 2mm diameter tube carrying a pulsatile flow, (b) In silico reproduction.

References

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Spontaneous chaotic oscillations at room temperature in a semiconductor superlattice model

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Fast spontaneous chaotic oscillations are used to generate high-quality true random sequences in random number generators. Using fast practical sources of entropy to produce true random sequences is crucial to make storage and transfer of data more secure at very high speeds [1]. Secure communications and e-commerce come to mind. While the first high-speed physical sources of entropy were chaotic semiconductor lasers [2], the discovery of spontaneous chaos in semiconductor superlattices at room temperature provides a valuable all-electronic nanotechnology alternative [3].

Analysis and numerical simulations of appropriate superlattice models are needed to understand spontaneous chaos at room temperature. So far, only idealized models of superlattices having identical periods have been studied. Spontaneous chaos in the current through the superlattice occurs when it is biased in narrow dc voltage ranges near sharp transitions between different current oscillation modes [4]. Internal shot and thermal noise enhances chaos [4]. When the superlattice is biased in a voltage region close to the transition between stationary and time periodic current, we have shown that external noise added to dc voltage bias may produce non-periodic chaotic current signals [5]. In addition, we will discuss different superlattices configurations that may enhance chaotic behavior [6].

References

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Modeling Electronic Properties of Twisted 2D Atomic Heterostructures

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Since the successful exfoliation of two-dimensional graphene and similar materials like transition metal dichalcogenides (TMDCs), van der Waals (vdW) materials have been increasingly studied as a new non-silicon platform for electronics and technology. Due to their layered "sheet"-like geometry, stacking vdW layers is suitable to study the interplay between different low-dimensional physics phenomenon. Treating the stacking order and orientation as experimental control knobs may lead to the creation of useful new materials. However, to understand the interaction between layers an accurate and transferable interlayer coupling model is needed. In our work, we map out an ab-initio tight-binding model for interlayer interactions by applying Wannier transformations to a survey of DFT results [1] [2]. We then apply our fitted tight-binding models to larger systems using both a periodic method (10^3 atoms) and a large-scale aperiodic method (10^6 atoms). For the periodic case, we have demonstrated Fermi velocity renormalizations, Van Hove singularities, flat bands and moire patterns in the electron density. We further investigate the electronic properties under commensurate magnetic field and the associated Chern numbers of the Landau levels. For the aperiodic method, our use of a locality formalism provides a new and clear vocabulary for understanding twisted systems in the context of local operators and atomic configurations. We show that our modeling successfully reproduces existing experimental knowledge for the electronic properties of twisted bilayer graphene, and discuss some predictions for the newer and less understood TMDC systems. This establishes the ab-initio Wannier tight-binding approach as an efficient and reliable method, applicable to general van der Waals heterostructures in the presence of magnetic fields and defects.

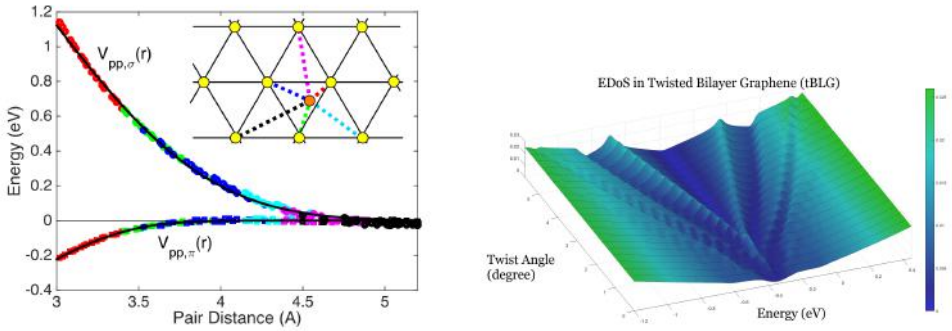

Figure 1: Left: Interlayer hopping terms in bilayer MoS_2. Right: Electronic Density of States for twisted bilayer graphene.

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The 2016 BIRS Workshop on Coupled Mathematical Models for Physical and Biological Nanoscale Systems and Their Applications,
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Towards multiscale modeling of incommensurate 2D van der Waals heterostructures

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Two-dimensional materials have generated a lot of interest in the past decade as a new toolbox for electronics [1]. This family includes insulators (boron nitride), semiconductors (transition metal dichalcogenides), and conductors (graphene). Vertical stacks of a few layers of such materials, interacting through van der Waals forces, create a venue to explore and tune desired mechanical and electronic properties. Numerical computations will be essential to explore the possibilites of such assemblies, such as tuning properties through the relative twist angle between layers, chemical doping, elastic stresses, etc. However, the generically incommensurate character of these systems represents a significant hurdle. Due to the lack of periodicity, many problems remain open in this field [2].

In this talk, we present some progress towards multi-scale calculations aimed at predicting macroscopic properties of heterostructures. First, we recall the electronic properties of monolayer 2D materials and the geometry of mono- as well as few-layers assemblies. Tight-binding models can be parameterized from ab-initio, micro-scale DFT calculations [3]. These models can then be used as reduced models for meso-scale numerical calculations. We present a perturbation approach which allows the computation of observables such as the density matrix in an incommensurate bilayer stacking. We also present some prospects for the calculation of transport properties in incommensurate stackings.

These results have been obtained in the framework of a collaboration with the groups of M. Luskin (Math, UofM), Efthimios Kaxiras (Physics, Harvard) and Eric Cancès (Ecole des Ponts).

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DNA, RNA and proteins in confined geometries: from precision medicine to new nanoscale phenomena

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Confining biological macromolecules - such as DNA, RNA and proteins - in channels of nanoscale dimensions offers unprecedented opportunities in "precision medicine", namely in our ability to tailor drugs to the specific genome/transcriptome/proteome of each individual [1,2]. In addition, this research is opening up the possibility of exploring physical properties and new phenomena of liquids and polymers in confined geometries that were not even conceivable a decade ago. As an example of the first research direction, I will show a novel technique for *de novo* protein sequencing that involves translocating a polypeptide through a synthetic nanochannel and measuring the ionic current of each amino acid through an intersecting perpendicular nanochannel [3]. The distribution of ionic currents for each of the 20 proteinogenic amino acids encoded by eukaryotic genes is found to be statistically distinct. I will then discuss phenomena that are analogous to those encountered in nanoscopic/mesoscopic physics, such as ionic Coulomb blockade [4], and ionic "quantized conductance" [5]. The first has been recently verified experimentally using MoS2 2-dimensional membranes [6], while the second leads to a universal mechanism for ion selectivity in graphene and other atomically thin pores [7].

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A multiscale moving contact line theory and its applications to dynamic droplet spreading and cell motility

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Durotaxis is a word used in biology to describe the spontaneous motion of adherent cells from soft to stiff regions. Recently, it is demonstrated that passive liquid droplets are also capable of sensing the stiffness of the substrate and migrate accordingly. Currently the investigations of these phenomena are mainly conducted through experiments.

The conventional hydrodynamics of the moving contact line (MCL) theory is easily considered to be a first choice in solving this type of problems. But the MCL theory suffers from its well-known incompatibility between the no-slip boundary condition, which states that there should no relative velocity between the liquid and solid at the interface. Also, it treats the substrate as a motionless boundary, which is not always the case. In this presentation, a multiscale moving contact line (MMCL) theory is going to be introduced, which is a seamless combination of a multiscale adhesive surface contact model and an interface model. The multiscale adhesive surface contact model characterizes the contact interaction between deformable bodies, by making use of surface traction induced by atomistic particle interactions. The adhesive contact forces levitate the droplet up so that the conventional no-slip condition can be employed free of contradiction. The interface model serves to capture the surface tension effect in the system, by introducing a series of interface dynamic equations of motion based on a surface elasticity theory.

The MMCL theory is first used to simulate dynamic droplet spreading on various substrates. Combined with a soft matter cell model, it is also employed to model the universal dynamics of cell spreading over elastic substrates. By assuming a linear dependence of the cell membrane actin tension on the substrate elasticity, the crawling phenomena of a cell on the substrate with varying rigidity is captured.

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Chaotic current self-oscillations in weakly coupled semiconductor superlattices for true random number generation

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A weakly coupled semiconductor superlattice (SSL) represents an almost ideal one-dimensional nonlinear dynamical system with a large number of degrees of freedom, the nonlinearity of which is due to sequential resonant tunneling between adjacent quantum wells. Fluctuations of the layer thicknesses, electron density, energy levels, and inter-well coupling transform a weakly coupled SSL into a complex nonlinear system, in which the electron transport is strongly dissipative. A great richness of nonlinear transport behavior has been observed in weakly coupled SSLs, including the formation of stationary electric-field domains, periodic as well as quasi-period current self-oscillations, and even driven as well as undriven chaos [1]. The oscillatory behavior is attributed to the localized, oscillatory motion of the domain boundary, which separates the high from the low electric-field domain. Only very recently, spontaneous chaotic [2] and quasi-periodic [3] current self-oscillations were observed at room temperature in GaAs/(Al,Ga)As SLs using an Al content of 45%, which results in the largest direct barrier for this materials system.

Based on these weakly coupled GaAs/$Ga_{0.55}Al_{0.45}As$ SLs operating at room temperature, an all-electronic true random number generator (TRNG) has been demonstrated [4]. The spontaneous chaotic current self-oscillations with large amplitudes characterized by a bandwidth of several hundred MHz do not require external feedback or conversion to an electronic signal prior to digitization. The fully electronic implementation suggests scalability and minimal post processing in comparison to existing optical implementations. The achievable bit rates of up to 80 Gbit/s are very competitive, being about two orders of magnitude larger than typical bit rates for currently available all-electronic TRNGs. Even more recently, the synchronization of chaos based on room temperature spontaneous chaotic current self-oscillations in a weakly coupled GaAs/$Ga_{0.55}Al_{0.45}As$ SL has been demonstrated as a useful building block for various tasks in secure communications, including a source of all-electronic ultrafast TRNG [5]. Several types of chaos synchronization have been experimentally demonstrated, in particular leader-laggard, face-to-face, and zero-lag synchronization in networks of coupled SSLs. The realization of chaotic SSLs without external feedback and the synchronization among different structured SSLs open up the possibility for advanced secure multi-user communication methods based on large networks of coupled SSLs.

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Predictive multiscale modeling of properties and interaction of macro/bio molecules in solvents and mixtures

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Over the past few decades nanoscience and molecular biology has shown a strong growth worldwide in many areas of research and proved their significance in todayś competitive environment. However, there still remains an enormous potential for further development which could revolutionize every area of human life. Unfortunately, in some cases, that potential is screened out by complexity and multilevel character of systems and processes at a nanometer scale. The success of future applications in a high-tech industry requires deep understanding of fundamental mechanisms on different levels of description and their communication. That could be provided only by appropriate combination of experimental study with predictive theoretical modeling. Nowadays, more and more scientists in different fields of chemistry and biology are using computational modeling methods in their research, either as a technique per se, or as a complement to experimental work. However, despite the increasing attention to computational nanoscience and biology the specificity of application of standard theoretical and computational modeling in nanotechnology and bioscience is complicated due to complexity of the systems of interest and needs to be discussed separately, especially in the view of multilevel representation of systems and processes on nanoscale. One of most important and demanding applications in computational chemistry is multiscale modeling of properties and interaction of macro/bio molecules in solvents and mixtures. The presentation will address different aspects of theoretical and computational approaches and their combination at the different time and length scales to model impact of solvents on physicochemical properties of molecules as geometry, conformational equilibria, reaction rates, as well as their UV-vis, IR, or NMR spectra. It will focus on the combination of statistical-mechanical molecular theory of liquids (3D reference interaction site model, known as 3D-RISM) with density functional theory (DFT) which provides the accurate and efficient way to predict the electronic properties of molecular system in different solvents and mixtures with high level of accuracy comparable with simulations but with less computational cost [1]. Similar to explicit solvent simulations, 3D-RISM properly accounts for chemical and physical activity of both solute and solvent molecules, such as hydrogen bonding and hydrophobic forces, by yielding the 3D site density distributions of the solvent. Moreover, it readily provides, via analytical expressions, the solvation thermodynamics, including the solvation free energy, its energetic and entropic decomposition, and partial molar volume and compressibility. Recently the number of new approaches and approximations was developed in order to increase efficiency of 3D-RISM and DFT combination. They could be subdivided into two main groups focused on the optimization of 3D-RISM algorithm (memory optimization, parallelization, etc.) and methodology improvements [2]. I will present a review and analysis of latest achievements focused on improves of accuracy and applicability the combination. Some examples will be also discussed.

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Multiphysics Models for the Bioelectronic Interface of Tethered Artificial Cell Membranes

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Tethered artificial cell membranes provide a stable platform for modelling the dynamics of biological membranes containing cytoskeletal supports, and can also be used for biosensing. Examples of such platforms include the: (i) the Ion Channel Switch (ICS) biosensor for detecting the presence of analyte molecules in a fluid chamber, (ii) the Pore Formation Measurement Platform (PFMP) for detecting the presence of pore forming proteins and peptides, (iii) the Controlled Electroporation Measurement Device (CED) that provides reliable measurements of electroporation phenomenon, and (iv) the Electrophysiological Response Platform (ERP) that measures the response of cells. These four tethered membrane based measurement platforms are all presented schematically in Fig.1. To capture the multi-spatial and multi-temporal processes present, coarse-grained molecular dynamics, continuum, and reaction-rate theory are used to model the tethered membrane and the bioelectronic interface. The models are validated using experimental measurements from the ICS, PFMP, CED, and ERP which include: measuring the pore formation dynamics of the antimicrobial peptide PGLa and the protein toxin α-Hemolysin; the ICS biosensor for measuring nano-molar concentrations of streptavidin, ferritin, thyroid stimulating hormone (TSH), and human chorionic gonadotropin (pregnancy hormone hCG); the CED for measuring electroporation of membranes with different tethering densities, and membrane compositions; and the ERP for measuring the response of the voltage-gated NaChBac ion channel, and the response of skeletal myoblasts which are attractive donor cells for cardiomyoplasty. The modelling methodology presented is essential for the design and operation of novel tethered artificial cell membrane devices for clinical diagnosis and biosensing.

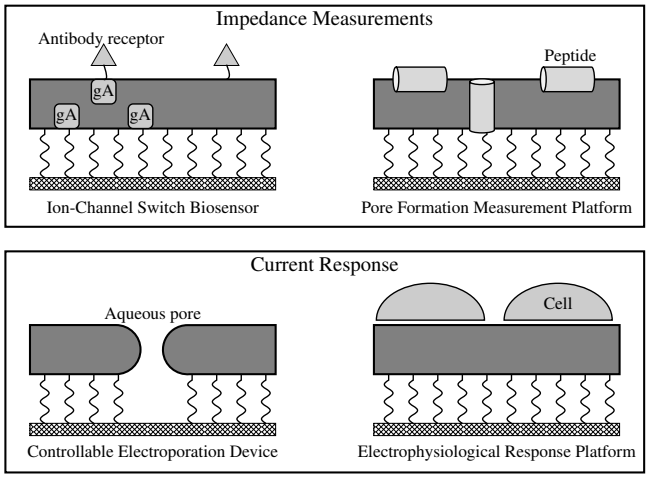

Figure 1: A schematic diagram of the ICS, PFMP, CED, and ERP tethered membrane devices. The tethered membrane is depicted in gray, and the gold interface by the crosshatch pattern. The unifying theme of all the devices is the use of an inert gold bioelectronic interface and an engineered tethered membrane.

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Non-perturbative approaches in nanoscience and corrections to finite-size scaling

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Non-perturbative approaches like Monte Carlo (MC) simulation and non-perturbative nonequilibrium Greens functions (NEGF) method become increasingly important in nanoscience. Particular applications cover description of charge transport and optical phenomena in nano-scale systems such as microelectronic devices, graphene layers, etc. Here we consider another application – behavior of small and large spin systems near the phase transition point, based on non-perturbative analytical evaluation of **k**-space integrals, as well as MC method. Lattice spin models are considered, where certain value of the spin variable is related to each lattice site. In the Ising model, the spin variable σ can take only one of two possible values ± 1. In the scalar φ^4 model, the spin variable φ can take any value within $-\infty < \varphi < \infty$. Such models exhibit second-order phase transition in the thermodynamic limit, where the linear lattice size L tends to infinity. The behavior of these models on finite lattices is described by the finite-size scaling. Moreover, the scaling behavior near the critical point can be remarkably varied depending on that whether small or large lattices are considered. This effect is described by corrections to the leading scaling behavior. Finite-size scaling and corrections to scaling are important to understand the difference in the behavior of very small nano-scale systems and large systems in the thermodynamic limit. Recently, corrections to scaling in the two-dimensional scalar φ^4 model have been studied based on our non-perturbative approaches [1]. Our arguments have shown the existence of nontrivial correction terms with the correction-to-scaling exponents $\omega_\ell < 1$ in the finite-size scaling of the 2D φ^4 model. Our analytical arguments predict $\omega \leq (\gamma - 1)/\nu$ for the leading correction–to–scaling exponent ω in the 2D φ^4 model and 3D φ^4 and Ising models, where γ and ν are the critical exponents of magnetic susceptibility and correlation length, respectively. It implies that ω has a remarkably smaller value $\omega \leq (\gamma - 1)/\nu \approx 0.38$ than the usually accepted ones about 0.83 [2] in three dimensions. We have performed MC simulations of the 3D Ising model for small, as well as large linear lattice sizes up to $L = 2560$, providing a numerical evidence for this challenging prediction. Our approach along with several other non-perturbative approaches reveals a potential application of non-perturbative methods to nanotechnology through condensed matter physics, e. g., semiconductor physics [3] and physics of disordered sytems like spin glasses [4].

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Dynamic models for Lipid Bilayers: from Biosensing to Electroporation

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We discuss and evaluate models for the dynamics of two novel measurement platforms: (i) a Pore Formation Measurement Platform (PFMP) for detecting the presence of pore forming proteins and peptides, (ii) the Ion Channel Switch (ICS) biosensor for detecting the presence of analyte molecules in a fluid chamber. Common to both measurement platforms is that they are comprised of an engineered tethered membrane. The electrical response is modelled using continuum theories for electrodiffusive flow coupled with boundary conditions for modelling chemical reactions and electrical double layers present at the bioelectronic interface. Experimental measurements are used to validate the predictive accuracy of the dynamic models.

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An Atomistic-to-Continuum Non-equilibrium Molecular Dynamics and Its Applications to Multiscale Coupling

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After more than twenty years research on multiscale simulations, a fundamental question still lingers: What is the statistical mechanics foundation of the multiscale simulation research?

To partially answer this question, in this presentation, we shall introduce a novel con-current multiscale micromorphic molecular dynamics (MMMD), which extends the equilibrium Andersen-Parrinello-Rahman molecular dynamics to non-equilibrium molecular dynamics systems with arbitrary finite-size domains. More importantly, MMMD takes the macroscale continuum boundary conditions as the inputs of microscale molecular dynamics, providing a top-down passage in microscale molecular dynamics simulations.

The multiscale micromorphic molecular dynamics is a con-current coupling of the microscale molecular dynamics with mesoscale and macroscale nonlinear continuum dynamics. By choosing proper statistical closure conditions, we have shown that the Andersen-Parrinello-Rahman molecular dynamics is a special case of the proposed multiscale molecular dynamics. In other words, we have shown that the Andersen-Parrinello-Rahman molecular dynamics can be rigorously formulated and justified from first principle. Moreover, the con-current multiscale continuum-molecular dynamics provides a solid theoretical foundation for non-equilibrium molecular dynamics, and one may be able to derive the basic equations of motions of nonlinear continuum mechanics from first principle molecular dynamics.

We have implemented this con-current multiscale dynamics formulation by developing a three-dimensional multiscale continuum-molecular dynamics computer code to simulate phase transformations in various crystalline solid materials. In this presentation, we shall present several numerical examples of the proposed MMMD to demonstrate its validity and apply the proposed MMMD to construct multiscale interphase zone to seamlessly couple Molecular Dynamics with Peridynamics to solve fracture and crack propagation problems.

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Analysis of rippling and commensurate-incommensurate transitions in one-dimensional coupled chains

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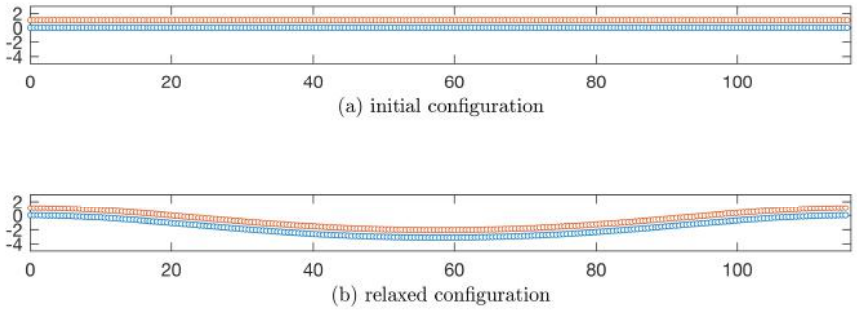
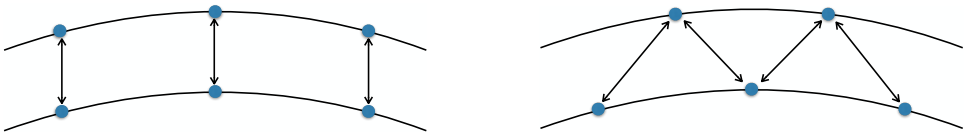
Graphene and other recently developed 2D materials exhibit exceptionally strong in-plane stiffness. Relaxation of few-layer structures, either free-standing or on slightly mismatched substrates occurs mostly through out-of-plane bending and the creation of large-scale ripples. In this work, we present a novel double chain model, where we allow relaxation to occur by *bending* of the incommensurate coupled system of chains. As we will see, this model can be seen as a new application of the well-known Frenkel-Kontorova model for a one-dimensional atomic chain lying in a periodic potential. We focus in particular on modeling and analyzing ripples occurring in ground state configurations, as well as their numerical simulation. We will also discuss the prospects for extensions to commensurate-incommensurate transitions in 2D heterostructures.



(a) initial configuration

(b) relaxed configuration

Figure 1: Numerical relaxation of coupled chains by the creation of ripples.



(a) Aligned atomic configuration

(b) Staggered atomic configuration

Figure 2: Local atomic configurations: aligned situation (a) leads to a higher energy contribution than the staggered configuration (b).

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Electronic Density of States for Incommensurate Layers

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Bloch theory provides an elegant solution for describing the electronic structure of periodic materials. However, there has been a lot of focus recently on the study of *incommensurate* layers of two-dimensional crystal structures [2]. In the absence of periodicity, computing the electronic structure of such materials becomes more difficult.

One common approach to approximate the electronic properties of such a system is to artificially strain it to obtain periodicity on a large supercell, and then apply Bloch theory to this periodic system [2]. Commensurate approximations to an incommensurate system quickly become expensive. We introduce and analyze a new method for computing a class of observables derived from the density of states for multi-layer incommensurate heterostructures *without* requiring an artificial strain in the system.

We use a tight-binding approximation, which approximates the Hamiltonian as a matrix over the lattice sites,

$$H_{R\alpha,R'\alpha'} = h_{\alpha\alpha'}(R-R'), \quad h_{\alpha\alpha'} \in C(\mathbb{R}^2).$$

Here R, R' are lattice site positions, and α, α' are orbital indices. We define an observable $g \in C(\mathbb{R})$ on the infinite system via a limit of finite cylindrical cut-outs of the system, H_r with radius r:

$$D[H](g) = \lim_{r\to\infty} \frac{1}{\alpha r^2} \mathrm{Tr}[g(H_r)],$$

where α is a normalization constant. The trace can be split so that we get the contribution from a single orbital:

$$D_{R\alpha}[H](g) = \lim_{r\to\infty} [g(H_r)]_{R\alpha,R\alpha}.$$

The infinite material can be approximated as an integral over orbital contributions, which is an integral over all possible relative shifts between the materials. A local orbital contribution can be approximated using a cylindrical cut-out of the material centered at the site of interest, and then a Kernel Polynomial Method can be applied [3]. The error can be analyzed using resolvent decay methods [1].

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Thermalized sheets and shells: Gaussian curvature matters

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Understanding deformations of macroscopic thin plates and shells has a long and rich history, culminating with the Foeppl-von Karman equations in 1904, characterized by a dimensionless coupling constant (the "Foeppl-von Karman number") that can easily reach $vK = 10^7$ in an ordinary sheet of writing paper. However, thermal fluctuations in thin elastic membranes fundamentally alter the long wavelength physics, as exemplified by experiments from the McEuen group at Cornell that twist and bend individual atomically-thin free-standing graphene sheets (with $vK = 10^{13}$!) We review here the remarkable properties of thermalized sheets, where enhancements of the bending rigidity by factors of ~ 5000 have now been observed. We then move on to discuss thin amorphous spherical shells with a uniform nonzero curvature, accessible for example with soft matter experiments on diblock copolymers. This curvature couples the in-plane stretching modes with the out-of-plane undulation modes, giving rise to qualitative differences in the fluctuations of thermal spherical shells compared to flat membranes. Interesting effects arise because a shell can support a pressure difference between its interior and exterior. Thermal corrections to the predictions of classical shell theory for microscale shells diverge as the shell radius tends to infinity.

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Geometry of Noise Driven Dynamical Systems

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In their book on path integrals, Feyman and Hibbs formulated a "geometrical optics" of most probable paths in stochastic dynamical systems. The most probable path in state space between two given endpoints minimizes a *stochastic action* functional. Some significant features of this geometric optics: The speed along the most probable path equals the deterministic speed, and generally speaking, the "Snell's law" that determines the geometry of the path is not invariant under orientation reversal. The paths from point a to point b, and from b back to a may be different. We present a dramatic example demonstrating the breaking of orientation reversal.

In the special cases with orientation reversal invariance, the stochastic dynamics is said to have *detailed balance*. The local expression of detailed balance is the vanishing of a *stochastic vorticity* tensor which is determined from the velocity field and noise tensor of the dynamics. A more traditional notion of detailed balance is based upon the existence of *equilibrium* solutions to the Folker-Planck equation, in which the probability current vanishes identically. The condition for equilibrium solutions in this sense is vanishing vorticity.

We can detect the breaking of detailed balance from direct measurements of stochastic trajectories: Project the dynamics down onto a two dimensional plane in state space, and look at the *area* swept out by the projected trajectory. If detailed balance is broken, there are planes of projection, so that the expected area grows linearly in time. We carry out this program for a simple RC network with "cold" and "hot" resistors. The breaking of detailed balance directly correlates with net heat transfer from the hot resistor to the cold resistor. One of the intriguing aspects of the area crtierion: We can implement it in practice, without knowledge of the velocity field and noise tensor of the stochastic dynamics.

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New Locality Results for the Tight Binding Model and Applications

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I will review results on the locality of interaction in the tight-binding model (treated as a toy-model for quantum chemistry). Specifically, I will make precise in what sense the *local density of states* (or, projected density of states) depends only locally on the environment of an atom.

With this understanding in hand a number of applications can be pursued which I will briefly summarise:

1. derivation of thermodynamic limit models for crystal defect (equivalence of canonical and grand-canonical ensemble) [3]
2. TB site energies and energy-based QM/MM hybrid models with rigorous error estimates [1, 2];
3. Regularity of the density matrix and tensor network expansion [5];
4. a generalisation of Brillouin-zone sampling to incommensurate layers of 2D lattices [4] (see also the talk by Daniel Massatt)

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Long Range Transport and Dark States in Quantum Dot Arrays

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Superpositions of indirectly coupled states are possible in quantum mechanics even when the intermediate states are far apart in energy. This is achieved via higher-order transitions in which the energetically forbidden intermediate states are only virtually occupied. Interest in such long-range transitions has increased recently within the context of quantum information processing with the possibility of low dissipation transfer of quantum states or coherent manipulation of two distant qubits .The recently achieved control and tunability of triple quantum dots allow to investigate phenomena relying on quantum superpositions of distant states mediated by tunneling. Recent experiments in these devices show clear evidence of charge and spin electron exchange between the outermost dots [1, 2, 3]. In the present talk I will discuss configurations of triple dots in series where long range transfer and quantum interferences determine the transport properties. I will show that the destructive interference between two virtual paths can lead to current cancelation, what we termed superexchange blockade[4]. Finally I will address long-range transport and quantum interferences in ac driven triple dots where transitions between distant and detuned dots are mediated by the exchange of photons[5]. We propose the phase difference between the two ac voltages as an external parameter, which can be easily tuned to manipulate the current characteristics. For gate voltages in phase opposition we find quantum destructive interferences among long-range and direct photon-assisted transitions, analogous to the interferences in closed-loop undriven triple dots. As the voltages oscillate in phase, interferences between multiple virtual paths give rise to dark states. Those totally cancel the current, and could be experimentally resolved.

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Path-space information metrics and variational inference for non-equilibrium coarse-grained systems

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We discuss information-theoretic tools for obtaining optimized coarse-grained molecular models for both equilibrium and non-equilibrium molecular dynamics. The presented approach compares microscopic behavior of molecular systems to para- metric or non-parametric coarse-grained systems using the relative entropy between distributions on the path space. It allows us to formulate a corresponding path space variational inference problem. The methods become entirely data-driven when the microscopic dynamics are replaced with corresponding correlated data in the form of time series. We also present results from [1, 3, 2].

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Coupling electromechanical effect in the optical properties of nanostructures

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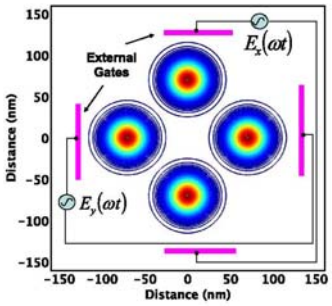
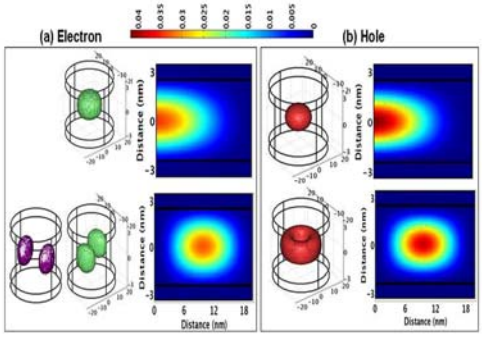
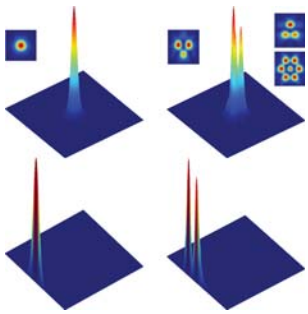
Our group is working on a mathematical treatment of the coupling effects (electromechanical, electric and magnetic fields, spin-orbit couplings) in the electronic properties of wide range of semiconductor materials. Such coupling effect in the band structures of semiconductor devices become more interesting topics in the coming decades to implement such coupling effects in the spintronic and transport properties of semiconductor devices including band gap opening in graphene. For example, we design the control pulse that can be applied in the gates to let the quantum states to move in a desired fashion that lead us to investigate interesting features of dynamical and geometric phases in the variety of semiconductor systems.

In Fig.1 (left panel), we showed the realistic design of GaAs quantum dots that moves adiabatically in the plane of two dimensional electron gas with the application of gate controlled realistic control pulse. Such adiabatic movement of the dots allow us to investigate the coupling effect of electric field, magnetic field and spin-orbit coupling in the geometric phase. In Fig.2 (middle panel), by utilizing strain dependent 8 band k.p theory, we investigate the coupling of electromechanical effect in the band structures of wurtzite GaN quantum dots. As can be seen, coupling effects can control the localized wave functions in a desired fashion. In Fig.3 (right panel), we investigate the coupling effect of thermo-electroelasticity theory in the band structures of grapheme quantum dots. The coupling effect clearly showed two distinct quantum modes, zigzag states at the zigzag boundary and localized states at the center of the graphene sheets.







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Pulling of biomolecules: lessons from toy models

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In recent years, atomic force microscopy (AFM) has been used to look into the elasticity of modular proteins, which comprise a certain number of identical protein domains [3]. The molecule is typically pulled from one end while the other is kept fixed, and either the length of the biomolecule or the force applied on it is controlled.

In the above experiments, the force-extension curve (FEC) is recorded, which gives the force needed to stretch the biomolecule as a function of its length. In modular proteins, the FEC shows a sawtooth behaviour under length-control: the unfolding of the different units that constitute the polyprotein is accompanied by a drop of the force. Moreover, the force at which the unfolding takes place, increases with the stretching rate [4–8].

On the other hand, there are also protein domains that are composed of several stable structural units or "unfoldons". The unfolding pathway is defined as the order and the way in which these "unfoldons" unravel, and it depends on the pulling speed. Consistently with the physical intuition, the weakest unfoldon opens first at low pulling rates. At higher rates, no longer is the first unit that unfolds but the pulled one [9–12].

In this talk, we discuss how some key aspects of these pulling experiments can be understood by using "toy" models [13–15]. Basically, the extension of each unit follows an overdamped Langevin equation. First, for the analysis of the FEC, the units are independent except for the global constraint given by the length-control condition. Second, we study the unfolding pathway by taking into account the spatial structure of the molecule, which introduces crucial additional couplings among the units.

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Signal and Information Processing with Biomolecules: Enzyme-Catalyzed Reactions and Their Cascades for Multi-Input Biosensing and Biocomputing

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Novel paradigms of signal and information processing have received significant attention based on their promise of new functionalities, new interfacing capabilities, and in some cases speed-up for sensor, diagnostic, and computational applications. Such "unconventional computing" realizations are in some cases contemplated as competitive, but in most situations will be complementary to the modern electronics technology.

An emerging research field of processing signals and information by using biomolecular processes will be surveyed in this talk, and specific examples and research results will be presented for enzyme-catalyzed biomolecular reactions. For additional information, see Ref. [1, 2, 3] and Fig. 1.

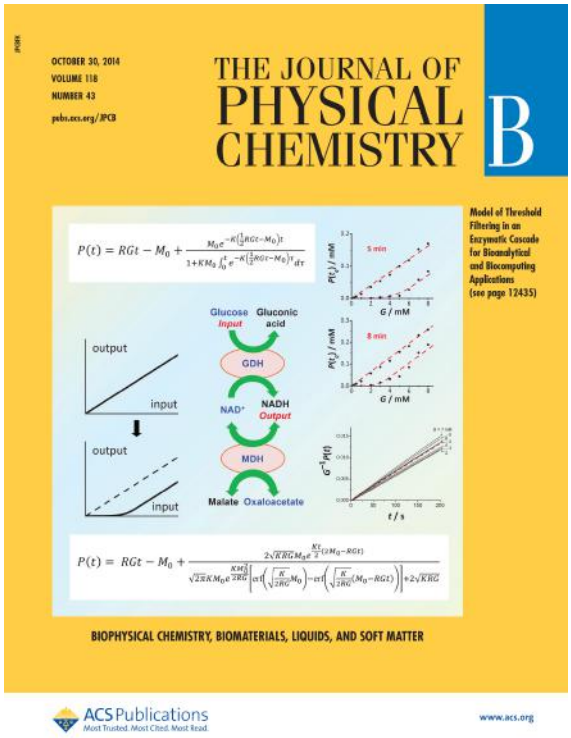

Figure 1: Issue cover showcasing our results, Ref. [2], highlighted by the journal editors.

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Moving under confinement

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How does confinement alter the transport properties of colloidal particles, the functionalities of molecular machines and in general the mechanisms of energy-transfer and energy-conversion at small scales? This question, fundamental for the modelling of soft-matter systems and biological systems, is attracting the interest of many researchers in the field. In a basic model proposed, the confinement effects are considered through an entropic potential. It has been shown that transport through entropic barriers or entropic transport exhibits peculiar characteristics very different from those observed when activation takes place through energetic barriers. In this talk, I will briefly review recent progresses in the study of entropic transport and its applications to soft-matter and biological systems. I will show that the confinement plays a very important role in the mechanisms of energy-conversion at the nanoscale, in particular in the functionality of molecular machines.

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STM driven transition from rippled to buckled graphene in a spin-membrane model

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We consider a simple spin-membrane model of buckling and rippling in graphene [1]. Related models involving coupling of a mechanical system to spins are [2, 3, 4]. Our model exhibits transitions from a flat but rippled membrane to a buckled rigid one. At high temperature the transition is second order but it is first order at low temperature for appropriate strength of the spin-spin coupling. Driving the system across the first order phase transition in conditions that mimic interaction of the graphene membrane with a Scanning Tunneling Microscope (STM) tip explains recent experiments [5]. Application of a voltage bias between the STM tip and the membrane has a twofold effect: (i) it induces a tunneling current that locally heats the sample, and (ii) it produces an electrostatic interaction between the tip and the sample. Experiments show that the suspended graphene sheet experiences a transition from "floppy" flat rippled to "rigid" buckled state [5]. In numerical simulations of our model, we observe a reversible behavior for small values of the STM current and an irreversible transition from flat rippled membrane to rigid buckled membrane when the current surpasses a critical value [1]. This work opens the possibility to test mechanical properties of graphene under different temperature and electrostatic conditions.

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Few Electron Triple Quantum Dot Circuits

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Few electron electrostatically gated quantum dots have been developed historically with two main purposes in mind. Firstly, they provide an excellent and controlled experimental laboratory for comparison with exact theoretical model calculations. Secondly, the versatility and tunability that results from having electrical control over the relevant quantum dot properties produced a potential platform for the development of spin based quantum computers and simulators. The materials in which the quantum dots are defined have important consequences for experiments via parameters such as those related to hyperfine, spin-orbit and electron-phonon coupling. The quantum dots described in this talk are defined in GaAs/AlGaAs heterostructures.

In this talk I will review some recent experiments we have performed on triple few electron quantum dots. A brief introduction will be provided about this genre of quantum dot devices and the techniques which have been developed to make measurements, e.g. how information about the spin state is obtained directly from charge measurements and how it is possible to identify the electron occupation of each quantum dot in an array. The emphasis on the talk will be on the surprisingly important and coherent role that phonons play in some of the measurements either directly or in combination with spin-orbit effects. A variety of experimental probes such as Landau-Zener-Stuckelberg-Majorana spin interferometry will be used to illustrate the effects.

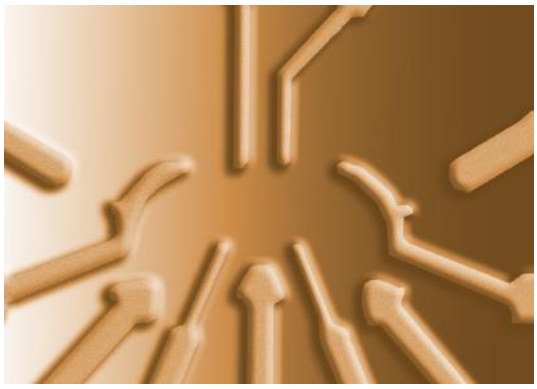

Figure 1: The gate layout used to define a few electron triple quantum dot potential used in the experiments

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Control of electronic heat flows in coupled quantum dots

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Electronic charge and heat flows can be separated in three-terminal conductors. Two terminals support the charge current with the third one serving as the heat source. The properties of the mesoscopic junction determine how the injected heat current affects the charge and energy transport in the conductor. This way, the system can be designed to work as a non-local heat engine (if heat is converted into useful power). This effect has been recently observed in coupled quantum dot configurations (cf. Fig. 1) where the heat transfer is mediated by electron-electron interactions [1, 2, 3, 4]. The magnitude and sign of the generated current can be controled by external gate voltages. They also allow one to manipulate the heat flows in all-thermal operations such as a thermal transistor or a thermal diode [5].

The non-local coupling to the heat sources of a non-thermalized state in the quantum dot also leads to the unprecedented occurrence of a thermoelectric response with no net absorbed heat [6].

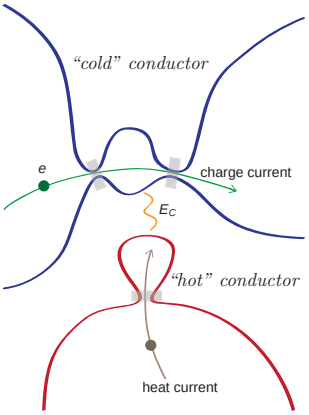

Figure 1: Sketch of a three-terminal quantum dot heat engine. Separation of charge and heat flows is achieved by the capacitive coupling of the charge conducting quantum dot and the one coupled to the heat source. The charging energy E_C parametrizes the energy transfer.

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August 28 - September 2, 2016

Numerical approximations of a mathematical model describing the evolution of nanoparticles in Ostwald ripening

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We propose numerical approximations to the solution of a general model that describes the growth and dissolution of a nanoparticle in a solution through energy driven Ostwald ripening on the particle surface. Precisely, we analyse the model for one nanoparticle consisting of a diffusion equation for the concentration of the solution and a Stefan problem for the evolution of the particle radius. We state the appropriate boundary conditions (fixed and moving) to take into account the nonlinear Ostwald-Freundlich condition, linking the concentration at the particle surface to the particle radius. We introduce a finite difference scheme in space and time incorporating the nonlinear moving boundary condition that approximates the evolution of the concentration of the monomer and the radius of the particle under a parabolic Courant-Friedrichs-Lewy stability condition.

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Self-consistent perturbation theory for two dimensional twisted bilayers

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Synthesis of vertically stacked two dimensional van der Waals heterostructures displaying a wide variety of applications is now possible with the advent of advanced experimental techniques. The properties of these heterostructures (and their applicability) are tunable with the relative orientation, lattice mismatch and separation between the layers. Theoretical modeling and simulation form a crucial part of the discovery and design of these materials, and provide important clues to the origin of exotic phenomena that may emerge in these heterostructures.

Analysis of these two dimensional van der Waals heterostructures with arbitrary angles of rotation between the layers involves unrealistically large and computationally expensive ab-initio calculations. To overcome this shortcoming, we have developed a model for weakly interacting heterostructures that treats the effect of one layer on the other as a perturbation, and restricts the calculations only to their primitive cells. Thus, circumventing the problem of computations over large supercells. We start by approximating the interaction potential between the twisted bilayers to that of a hypothetical configuration (viz. ideally stacked untwisted layers [1]); and then proceed to self-consistently calculating the charge density and hence, the interaction potential of the heterostructures. In this work, we test our model for bilayers of various combinations of graphene, hexagonal boron nitride and transition metal dichalcogenides, and discuss the advantages and shortcomings of the self-consistently calculated interaction potential of the heterostructures.

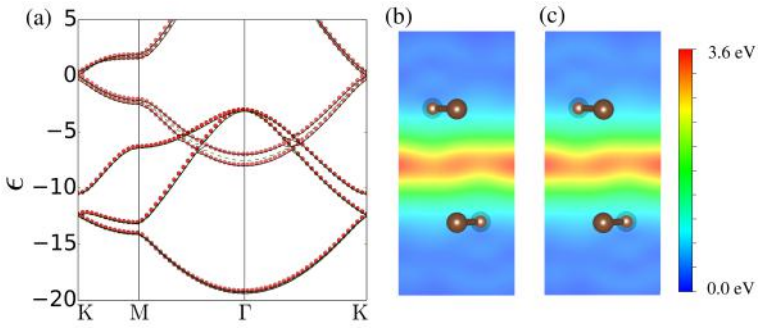

Figure 1: (a) Electronic band structure and interaction potential between the layers (b) from Density Functional Theoretical calculations and (c) self-consistently determined using perturbative approach of ideally AB stacked bilayer graphene. In panel (a), red dots are the results of self-consistent perturbation approach, solid lines and green dashed lines are the Kohn-Sham eigenvalues of bilayer and isolated layers respectively. Brown circles represent carbon atoms in (b) and (c).

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Microtubule I-V Characteristics Are Consistent with Memristor-like Behavior

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Memristors represent the fourth element of the electrical circuits complementing resistors, capacitors and inductors. Postulated to exist several decades ago, only recently examples of memristive behavior have been shown to occur by involving complicated semiconductive constructs. Hallmarks of memristive behavior include pinched and frequency-dependent I-V hysteresis loops and most importantly a functional dependence of the magnetic flux passing through an ideal memristor on its electrical charge. In this paper we provide theoretical and experimental evidence that specific biological protein polymers, namely microtubules, act according to the definition of a memeristor. Their biophysical properties lead to pinched hysteretic I-V dependence as well a classic dependence of magnetic flux on charge. Based on the information about the structure of microtubules we provide an estimate of memristance and discuss its significance for biology and nanotechnology.

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Onsager Principle for generalized hydrodynamic models and applications to cell migration

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I will first discuss a general modeling framework consisting of the variational approach together with the generalized Onsager principle for nonequilibrium processes. In this modeling approach, we first identify the internal variables for the microstructure in addition to the material density and velocity. Then, we calculate the total energy dissipation rate to derive the constitutive equations for the generalized hydrodynamic models. I will illustrate the idea using a few examples.

For the models so derived, we then develop efficient energy stable schemes based on their variational and dissipative structure. Once again, I will discuss a few examples from multiphase fluid flows to liquid crystals. Then, we present a couple of examples where the model and the numerical schemes are employed to develop tools to study cell migration and other cell dynamic behavior.

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Acoustic and optical phonon field couplings in piezoelectric semiconductors

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The properties and interaction between optical and acoustic phonon fields are important to assess dissipation mechanisms of quantum electronic systems as they determine the mechanical, thermal, and electrical properties of solids. Usually electron-phonon interactions lead to performance degrading of devices but they may also open up possibilities to tune device characteristics by virtue of material and geometry design.

Some cases of phonon tuning applications have been demonstrated in the context of population inversion in piezoelectric InGaAs quantum dot systems [1]. Some other recent phenomena where optical and acoustic phonon interactions are central include dissipation mechanisms in $2D$-based electronic and optical devices [2]. Determination of phonon fields and dispersion relations in many of the important semiconductor materials ($3D$ GaAs, GaN, ZnO and $2D$ MoS_2 and BN) require a full accountance of crystal anisotropy and inversion-asymmetry effects including piezoelectricity.

We present a self-contained and combined continuum elastic description of the couplings between acoustic and optical phonons in zincblende piezoelectric media [3] and also discuss phonon properties in $2D$-based materials such as graphene.

To simplify the problem we take a cubic piezoelectric slab as example and demonstrate that phonon modes always involve coupled acoustic and optical fields except when the phonon in-plane wavenumber component vanishes. This coupling between acoustic and electric fields also implies that acousto-optical phonons cannot exist at the LO phonon frequency where the dielectric constant vanishes. Finally we show that confined acousto-optical phonon modes cannot exist at any frequency in a piezoelectric slab. The equation framework is the elastic equations and the Maxwell-Poisson equation of a piezoelectric cubic material supplemented by boundary conditions at the slab interface. In this way a complete set of differential equations and boundary conditions is found that allows the lattice displacements u_x, u_y, u_z and the electric potential ϕ to be determined.

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Predictive Coarse-Graining

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We discuss a data-driven, coarse-graining formulation in the context of equilibrium statistical mechanics. In contrast to existing techniques which are based on a fine-to-coarse map, we adopt the opposite strategy by prescribing a probabilistic coarse-to-fine map. This corresponds to a directed probabilistic model where the coarse variables play the role of latent generators of the fine scale (all-atom) data. From an information-theoretic perspective, the framework proposed provides an improvement upon the relative entropy method that quantifies the uncertainty due to the information loss that unavoidably takes place during the CG process. Furthermore, it can be readily extended to a fully Bayesian model where various sources of uncertainties are reflected in the parameters' posterior. The latter can be used to produce not only point estimates of fine-scale reconstructions or macroscopic observables, but more importantly, predictive posterior distributions on these quantities. These quantify the confidence of the model as a function of the amount of data and the level of coarse-graining.

The issues of model complexity and model selection are seamlessly addressed by employing a hierarchical prior that favors the discovery of sparse solutions, revealing the most prominent features in the coarse-grained model. A flexible and parallelizable, Monte Carlo - Expectation-Maximization (MC-EM) scheme is proposed for carrying out inference and learning tasks. A comparative assessment of the proposed methodology is presented for a lattice spin system and the SPC/E water model.

This is a joint work with Markus Schöberl and Phaedon-Stelios Koutsourelakis, Technical University of Munich.

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Inelastic light scattering study of nanomotors caused by coherent energy transfer of photoexcited energy in hybrid inorganic-organic complexes

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The structure of the deoxyribonucleic acid (DNA) molecule is one of the most important for life and most fascinating biopolymers. In addition its central role as carrier of genetic information and translation of the genetic code into amino acid sequences of proteins, DNA holds great promise as a functional nanomaterial for broad bioanalysis applications, DNA computing, DNA nanotechnology, and early nanomedical diagnostics. Self-assembled semiconductor quantum dots (QDs) have received considerable attention as robust solid-state single photon emitters in a wide range of applications from fundamental studies of light-matter interactions to emerging fields of nanophotonics quantum information technology.

We will develop an inorganic-organic, electrostatic strategy that allows for the scalable self-assembly precisely placement and functionalization of individual nanoparticle by DNA single molecule. Because of the exquisite sensitivity of the vibrational mode frequency to the local chemical bonds generated by the surrounding atoms and molecules, high resolution Raman scattering provides a unique fingerprint for particular molecule or atomic arrangement and their interaction with the local environment. In this case the novel acquired properties of the complex can depend not only on the QD's intrinsic electronic structure but also its local environment. The self-assembly properties of individual semiconductor nanometer-sized quantum dots which confine electrons in all three directions are dominated by quantization in all three directions and as an individual real atom has a set of discrete energy levels on the example of functionalized QDs$-$DNA periodic complexes show switchable and optically traceable DNA molecular nanomotors. To illustrate the broad applicability of this method the fabrication and integration technique has been introduced with individual nanocrystalline nc$-$Si/SiO_2 QDs directly functionalized by single strand short oligonucleotides d($5^{'}20G$, $20T-3^{'}$). Here G is guanine and T is thiamine nucleotidies. Desighed label-free approach could be applied to diamond and other nanoparticles with versatile tailored properties. This DNA-based nanomotors strategy allows control over the distribution density of the motor moieties of the photoexcited carriers between non-organic in nc-Si/SiO_2 QDs localized Wanie-Mott exciton and Frenkel exciton of LUMO and HOMO states with nanometer precision. This is essential for the high efficiency of the system and for the generation of complex multi-responsive materials. Given the simplicity of this approach as well as the practical and scientific advantages, it can be of interest in a wide range of applications from fundamental studies of light-matter interactions to broad emerging research fields of nanophotonics and metamaterials that are closely interlinked. The selective switching of different coherent pathways between two well-defined conformational states, is triggered by a specific hybridization event, which induces a linear translational movement, observable by energy transfer Raman microspectroscopy.

We will show that such a coherent energy transfer process can be realized not only for free atoms and molecules, but in the hybrid functionalized semiconductor QD-DNA complex as well being very interesting for many important fundamental investigations of strong light-matter interactions and nanobiomedical applications.

Models of emergent networks

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In this talk, we will present a modelling framework for the emergence of networks and their evolution. We will provide various examples of such emergent networks: ant trails, extracellular fibers and blood capillaries. We believe this framework can apply to other types of networks in which the topology and topography of nodes and links is fuzzy and evolutive.

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Designing assembly strategies for efficient bacterial origami designs

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Recent advances in synthetic biology have expanded the ability to design tailored microorganisms for industrial and research purposes [1]. The efficiency of bacterial consortia as organized communities of purpose-designed individuals to develop complex chemical transformations [2] is limited by the spatial arrangement of the individuals, leading to poor efficiencies not valid for biotechnological applications.

In this work we present the '*bacterial origami*' approach as an integral strategy to solve this inconvenient. By using modified bacterial strains with the ability to assemble by pairs, we characterize and detail both computational and experimentally the dynamics of the spontaneous assembly process observed in the laboratory starting from randomly mixed individuals. Our results showed the formation of families of aggregates with a size distribution following a lognormal behaviour and showing a fractal-like pattern in their geometry as the size is increased. The effect of other variables related with the assembly process are also evaluated and discussed.

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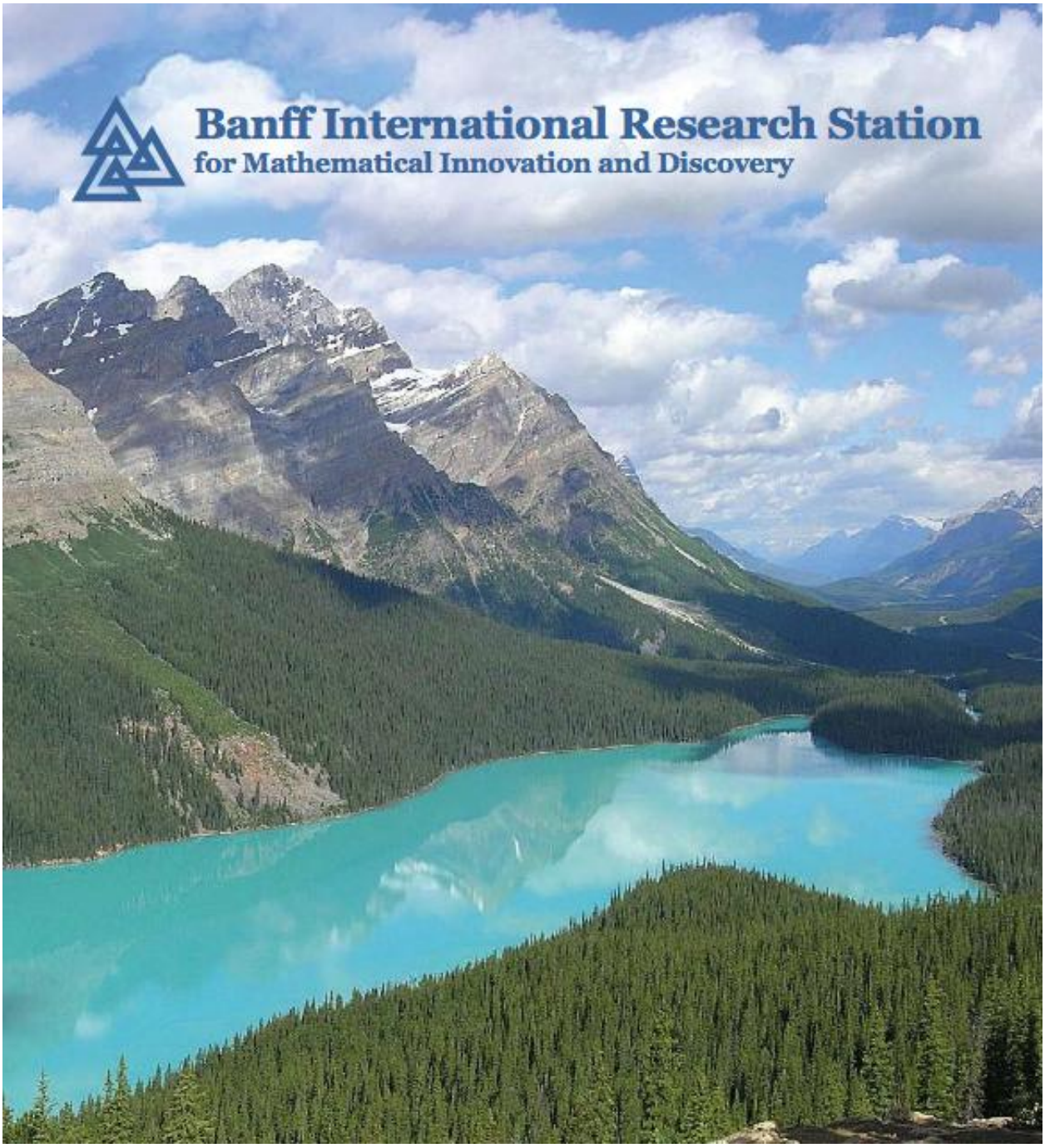
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