



# Particle-based methods in materials science

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## Abstracts

### Tapio Ala-Nissilä

#### *Multiscale modelling of graphene from nano to micron scales with the phase-field crystal model*

Over the last few years novel two-dimensional materials and nanoscopically thin heteroepitaxial overlayers have attracted intense attention due to their unusual properties and important technological applications. Many physical properties of these systems such as thermal conductivity and electrical transport are intimately coupled to the large scale mechanical and structural properties of the materials. However, modeling such properties is a formidable challenge due to a wide span of length and time scales involved. In this talk, I will review recent significant progress in structural multi-scale modeling of two dimensional materials and thin heteroepitaxial overlayers [1], and graphene in particular [2], based to a large extent on the Phase Field Crystal (PFC) model combined with standard microscopic modeling methods (classical Molecular Dynamics and Quantum Density Functional Theory). The PFC framework allows one to reach diffusive time scales for structural relaxation of the materials at the atomic scale, which facilitates quantitative characterisation of domain walls, dislocations, grain boundaries, and strain-driven self-organisation up to almost micron length scales. This allows one to study e.g. thermal conduction and electrical transport in realistic multi-grain systems [3].

References:

[1] K. R. Elder et al., Phys. Rev. Lett. vol. 108, 226102 (2012); Phys. Rev. B vol. 88, 075423 (2013); J. Chem. Phys. 144, 174703 (2016).

[2] P. Hirvonen et al., Phys. Rev. B 94, 035414 (2016).

[3] Z. Fan et al., Phys. Rev. B vol. 95, 144309 (2017); Nano Lett. 7b172 (2017); K. Azizi et al., Carbon 125, 384 (2017).

### Andrew Archer

#### *Density functional theory and dynamical density functional theory for classical many body systems*

I will introduce density functional theory (DFT) and dynamical density functional theory (DDFT) for classical many body systems. I will explain the fundamental ideas of DFT and DDFT, illustrating what types of systems are best described these theories and relating DFT/DDFT to other possible methods relevant in materials science.

### Rainer Backofen

#### *Modeling of ferromagnetic material with phase field crystal (PFC) and implication on interface movement*

Ferromagnetic materials undergo spontaneous magnetization. That is, microscopically defined magnetic moments align locally and may form macroscopic domains. Crystalline symmetry of the material breaks the rotational symmetry and lead to preferred direction of magnetization.

We apply the PFC model for multiferroic materials [1] for ferromagnetic materials in strong external magnetic fields. We discuss the properties of this model and show the influence of external magnetic fields on the movement of grain boundaries in different set ups. The results are analyzed with the macroscopic theory of interface evolution by mean curvature and a driving force due to the energy difference in bulk phases. We highlight that the microscopic structure of the PFC model and show the implication on the movement on interfaces. This leads to non-trivial macroscopic mobilities of grain boundaries. Additionally, we show that an external magnetic field breaks the

symmetry defined by the crystalline structure and the velocity of the grain boundary becomes dependent on the orientation of the magnetic field.

[1] Seymour et al, PRB 92, 184109 (2015)

### **Abhijit Chatterjee**

#### *Temperature programmed molecular dynamics: theory and applications*

Temperature programmed molecular dynamics (TPMD) method is a recently developed rare event acceleration scheme. TPMD can be used to efficiently study the long timescale dynamics of a material system. A situation commonly encountered in several complex materials is that the system remains trapped for long periods of time in a collection of potential basins in the energy landscape, called a superbasin. Transitions between superbasin states can be rare at molecular dynamics timescales, however, escapes from the superbasin involving larger activation barriers are even rarer. Often, it is the latter type of moves that are of interest when long timescales of seconds and beyond need to be accessed. TPMD method employs a temperature program with state-constrained molecular dynamics calculations that allows transitions of interest to happen more frequently. Separation of timescales is exploited for identifying the superbasin and selecting a superbasin escape for a move. Using TPMD method one can accurately study superbasin-to-superbasin transitions while disregarding low-barrier pathways that have been traditionally difficult to handle with rare-event simulations. I will describe some of the other key features of the TPMD method such as estimation of Arrhenius parameters for kinetic pathways. Application of the technique to various materials problems will be discussed.

### **Huajie Chen**

#### *QM/MM methods for crystalline defect*

We develop and analyze QM/MM (quantum/classic) hybrid methods for crystalline defects within the context of the tight-binding model. QM/MM methods employ accurate quantum mechanics (QM) models only in regions of interest (defects) and switch to computationally cheaper interatomic potential molecular mechanics (MM) models to describe the crystalline bulk. We propose new energy-based and force-based QM/MM methods, building on two principles:

- (i) locality of the QM model; and
- (ii) constructing the MM model as an explicit and controllable approximation of the QM model.

This approach enables us to rigorously establish convergence rates in terms of the size of the QM region. This is a joint work with Christoph Ortner.

### **Gabor Csanyi**

#### *The new dawn of force fields*

To follow

### **Genevieve Dusson**

#### *Permutation-invariant data-driven interatomic potentials*

For many applications *ab initio* computations are too expensive, so that interatomic potentials, often cheap to compute but less accurate, are in use. Originally derived from empirical models, these potentials have over the past few years mainly been developed from machine-learning methods.

In this talk, I will present an interatomic potential combining a data-driven approach with physically motivated functional forms – the many-body expansion. I will notably report our initial experiences with a practical implementation, describing in particular the roles of symmetries and of regularisation.

### **Ken Elder**

#### *Modelling microstructure formation using phase field crystal models*

Phase field crystal (PFC) models were originally developed as a simple way to incorporate the influence of elasticity and dislocations in material processing phenomena such as epitaxial and polycrystalline growth. These models were developed to explicitly recover well known results in the long-wavelength limit. In this regard I would like discuss how, in the small deformation limit, PFC models reduce to traditional phase field models and continuum elasticity theories. Furthermore I would outline recent extensions that were developed to such improve and extend the approach.

## Jim Evans

### *Stochastic particle-level modeling of coarsening: Cluster diffusion and coalescence on surfaces*

Stochastic particle-level lattice-gas models have enabled detailed characterization of the formation of non-equilibrium distributions of islands (also described as nanoclusters) during submonolayer deposition on flat surfaces, as well as their subsequent coarsening. For island formation, fundamental open questions remain regarding the size distribution and spatial distribution of islands (the latter including tessellation of the surface into capture zones surrounding islands). Post-deposition coarsening reduces the number of islands and increases their mean size, thereby evolving the system to equilibrium. This process can occur either via Ostwald Ripening (where small islands dissolve) or via Smoluchowski Ripening (i.e., diffusion and coalescence of islands). We focus on the latter processes where both diffusion and coalescence are mediated by periphery diffusion (PD) of atoms around the edge of the cluster. We utilize both tailored models and *ab initio* based models to describe the relevant PD kinetics. For the size-dependence of cluster diffusion, we find remarkably rich behavior on the nanoscale (with nucleation-mediated and facile branches of diffusion, strong oscillations in size) giving way to macroscopic behavior described by continuum Langevin theory.

## Ben Goddard

### *Dynamic density functional theory: modelling, numerics and analysis*

In recent years, a number of dynamic density functional theories (DDFTs) have been developed to describe colloid particle dynamics. These DDFTs aim to overcome the high-dimensionality of systems with large numbers of particles by reducing to the dynamics of the one-body density, described by a PDE in only three spatial dimensions, independent of the number of particles. The standard derivations start from stochastic equations of motion, but there are fundamental differences in the underlying assumptions in each DDFT. I will begin by giving an overview of some DDFTs, highlighting the assumptions and range of applicability. Particular attention will be given to the inclusion of inertia and hydrodynamic interactions, both of which strongly influence non-equilibrium properties of the system. I will then demonstrate the very good agreement with the underlying stochastic dynamics for a wide range of systems, including confined systems with hydrodynamic interactions. If time allows, I will also discuss an accurate and efficient pseudospectral numerical code that we have developed, as well as the passage to Smoluchowski-like and Navier–Stokes-like equations in appropriate limits. Joint work with Serafim Kalliadasis, Greg Pavliotis, and Andreas Nold

## Laszlo Granasy

### *Nucleation modes and polycrystalline growth in a hydrodynamic phase-field crystal model*

Nucleation of solid phases in undercooled liquids is investigated using a hydrodynamic model of solidification based on combining the phase-field crystal model with fluctuating nonlinear hydrodynamics [1, 2]. Structural aspects of homogeneous and heterogeneous nucleation will be addressed, including growth front nucleation mechanisms that lead to the formation of differently oriented grains at the solidification front in highly non-equilibrium liquids. It is predicted that even in simple liquids, amorphous precursor structures may assist crystal nucleation. It will be shown furthermore that new orientation may form at the perimeter of growing crystals by two mechanisms: via

- (i) incorporating dislocations into the crystalline phase during rapid solidification, and
- (ii) the interference of extended density waves ahead of the crystallization front observed in the vicinity of the stability limit of the liquid.

Joint work with Frigyes Podmaniczky and Gyula I. Tóth.

[1] G.I. Tóth et al. J. Phys.: Condens. Matter. 26, 055001 (2014).

[2] F. Podmaniczky et al. Phys. Rev. E. 95, 052801 (2017).

## Zhi-Feng Huang

### *Continuum field modeling of crystalline microstructures: length scales and bond-angle control*

The coarse-graining, density-field based continuum theories have been proven efficient in modeling complex material systems, particularly those involving multiple spatial and temporal scales. There are some fundamental but challenging issues that remain to be resolved, two of which will be discussed in this talk based on the phase field crystal type method:

- (i) how to systematically model and control the interparticle bond orientation in a continuum description, and
- (ii) how to address the coupling among microscopic and mesoscopic length scales.

For the first issue we construct an angle-adjustable density field formulation to simultaneously incorporate the micro-scale interparticle bond-angle anisotropy and the global-scale rotational invariance of material systems. This is achieved by making use of a decades-old mathematical concept/theorem of isotropic Cartesian tensor, and via the complete expansion of particle direct correlation functions particularly that of four-point correlation. Various 2D and 3D crystalline phases are modeled by this generic approach, which also shows the capability of continuous bond angle control and tuning. For the second issue of length scale coupling, it is addressed through a sample system of alloy liquid-solid interface and the development of a nonadiabatic amplitude equation formulation. The interface lattice pinning effect during material growth and effects of compositional stress on anisotropic interfacial properties are identified, as a result of meso-micro and meso-meso scale couplings

### **Tom Hudson**

#### *A rigorous approach to describing the mobility of screw dislocations*

Discrete Dislocation Dynamics (DDD) is a phenomenological modelling and simulation technique used to study plasticity in crystalline solids on length- and timescales inaccessible with molecular dynamics. In this talk, I will present some mathematical results demonstrating that in certain parameter regimes, forms of DDD for screw dislocations can be derived from a microscopic stochastic model.

### **Tony Lelievre**

#### *Metastability: a journey from stochastic processes to semiclassical analysis*

A stochastic process is metastable if it stays for a very long period of time in a region of the phase space (called a metastable region) before going to another metastable region, where it again remains trapped. Such processes naturally appear in many applications, metastability being related to a two time scale mechanism: the small time scale corresponds to the vibration period within the metastable regions and the large time scale is associated with the transitions between metastable states. For example, in molecular dynamics, the metastable regions are typically associated with the atomic conformations of a molecule (or an ensemble of molecules), and one is actually interested in simulating and studying the transitions between these conformations.

In this talk, I will explain how the exit events from a metastable state can be studied using an eigenvalue problem for a differential operator. This point of view is useful to build very efficient algorithms to simulate metastable stochastic processes (using in particular parallel architectures). It also gives a new way to prove the Eyring–Kramers laws and to justify the parametrization of an underlying Markov chain (Markov state model), using techniques from semiclassical analysis.

Reference: <https://arxiv.org/abs/1706.08728>

### **Stela Makri**

#### *A preconditioning scheme for minimum energy path finding methods*

In transition state theory, the study of thermally activated transitions between energy minima is achieved by finding transition paths connecting the minima. These paths provide information on the energy barrier and reaction rates of the system without going through long and expensive simulations. To find them, current techniques use steepest descent-like minimisation to relax a discretised initial guess. However, steepest descent typically gives slow convergence rates in the presence of ill-conditioned potentials. In this talk I will be discussing how to reduce the condition number of the potential of an arbitrary system and improve the convergence speed and robustness of transition path finding methods, using a preconditioning scheme. Our key assumption is that the cost of constructing a preconditioner is much smaller than the cost of computing the potential; for density functional theory the cost of single point evaluations is much more expensive than the computation of a preconditioner and thus the proposed approach improves computing times significantly. We have developed a preconditioning scheme, where the preconditioner acts as a coordinate transformation of the discrete images along the path to aid the ill-conditioning in the transverse direction and a preconditioning scheme that considers the interactions between the

images is currently in development. Finally, we are working towards a preconditioning scheme for finding energy barriers in hybrid quantum mechanical–molecular mechanical models.

### **Charalambos Makridakis**

#### *Formulation and analysis of discontinuous interface atomistic-continuum coupling methods*

A new class of atomistic-continuum coupled methods for crystalline materials, based on a discontinuous formulation of the interface terms, is presented and analysed. Error bounds for the energy and the first variation of the models are derived.

### **Simiso K. Mkhonta**

#### *Emergence of disordered hyperuniform systems in random pinning potentials*

Disordered hyperuniform materials are a novel class of amorphous systems that possess hidden long range order that manifest through the suppression of density fluctuations at large length scales. These materials have isotropic properties like an ideal gas or liquid, yet they exhibit energy band-gaps like crystals. In this talk, I will present results from the phase field crystal approach that demonstrate that random pinning potentials may be used to induce disordered hyperuniform states in binary phase materials and in two-dimensional crystalline materials. The development of methods for designing disordered hyperuniform materials is a field of tremendous interest because of the broad technological applications of these materials in photonics and related areas.

### **David Montiel**

#### *A three-dimensional phase-field crystal model for two-dimensional materials*

We introduce a Phase-Field Crystal (PFC) model to simulate the growth of 2D materials in three dimensions. Our approach employs a two-point correlation term in the free energy functional that is designed to energetically favor structures with periodicity along a plane but that are localized in the direction perpendicular to that plane. We show how this method can be applied to stabilize one-dimensional structures in two-dimensional systems and two-dimensional structures in three-dimensional system. In addition, we demonstrate the capability of the model to study three-dimensional effects, such as buckling of strained layers. This method extends the capability of the PFC model to the study of three-dimensional phenomena in 2D materials such as out-of-plane buckling around defects. Joint work with Guanglong Huang, Eli Alster, Peter Voorhees and Katsuyo Thornton.

### **Danny Perez**

#### *Strategies for optimal construction of Markov chain representations of atomistic dynamics and their application to irradiated materials*

A common way of representing the long-time dynamics of materials is in terms of a Markov chain that specifies the transition rates for transitions between metastable states. Such chains can either be analyzed directly, used to generate trajectories using kinetic Monte Carlo, or upscaled into mesoscale models such as cluster dynamics. While a number of approaches have been proposed to infer such a representation from direct molecular dynamics (MD) simulations, challenges remain. For example, as chains inferred from a finite amount of MD will in general be incomplete, quantifying their completeness is extremely desirable. In addition, making the construction of the chain as computationally affordable as possible is paramount. In this work, we simultaneously address these two questions. We first quantify the local completeness of the chain in terms of Bayesian estimators of the yet-unobserved rate, and its global completeness in terms of the residence time of trajectories within the explored subspace. We then systematically reduce the cost of creating the chain by maximizing the increase in residence time against the distribution of states in which additional MD is carried out and the temperature at which these are respectively carried out. Using examples of defects that are relevant to the evolution of irradiated materials, we demonstrate that our approach is an efficient, fully automated, and massively-parallel scheme to efficiently explore the long-time behavior of materials.

## **Marco Salvalaglio**

### *Coarse-grained, three-dimensional modeling of defect networks by the amplitude expansion of the phase field crystal model*

Extended defects, such as dislocations and grain boundaries (GBs), deeply affect macroscopic properties of crystalline materials, while their nature, motion, and reaction, strictly depend on microscopic features. The Phase-Field Crystal (PFC) allows for the study of GBs by focusing on the dynamics of the local atomic probability density on diffusive time scales [1]. However, it requires a fine spatial discretization, which limits the application of this method to relatively small systems. The amplitude expansion of the PFC (APFC) enables the study of larger systems, as it accounts for the evolution of the slowly varying (complex) amplitudes of the atomic probability densities [2]. We illustrate the modelling of defect networks at GBs forming between tilted/twisted crystals by means of the APFC model in two- and three-dimensions. This is achieved thanks to the implementation of the APFC equations within a Finite Element Method with advanced numerical features such as adaptive mesh refinement [3]. Dislocation networks at planar and spherical grain boundaries are shown for different lattice symmetries, namely triangular/honeycomb in 2D as well as body-centered cubic and face-centered cubic in 3D [4]. The dynamics of dislocation networks forming at spherical grain boundaries is also addressed, reproducing the anisotropic shrinkage of spherical grain and revealing general qualitative features independent of the specific rotational axis and crystal symmetry [4]. An extension of the classical model to control the energy of defects and GBs is also illustrated [3]. Moreover, we show the derivation of continuous deformation fields from complex amplitudes and discuss the comparison with continuous elasticity and atomistic modelling.

[1] K. R. Elder et al Phys. Rev. Lett. 88, 245701 (2002)

[2] N. Goldenfeld et al Phys. Rev. E 72, 020601 (2005)

[3] M. Salvalaglio, et al Phys. Rev. E 78, 184104, (2017)

[4] M. Salvalaglio, et al Phys. Rev. Materials 2, 053804 (2018)

## **Dimtri Schebarchov**

### *Structure optimization for clusters of particles*

In this talk I will juxtapose two themes:

- (1) theoretical structure prediction for atomic clusters, bound by an empirical potential; and
- (2) computational design of colloidal clusters with a desired optical response, described within classical electromagnetic theory.

While these two themes focus on different aspects of physics (which will be summarized here), they both involve optimizing the constituent particles' coordinates with respect to a given objective function. I will discuss a generalized basin-hopping (GBH) approach to global optimization, with some recent applications in theme 1, and then I will explore how GBH could be used in theme 2.

## **Tim Schulze**

### *Lattice and off-lattice kinetic Monte Carlo*

In this talk I will discuss the contrasting capabilities of lattice- and off-lattice kinetic Monte Carlo simulation, illustrating each with a particular application. For lattice based simulation I will consider the role of surface energy anisotropy in stabilizing the Bales-Zangwill meandering instability of step-flow. I will also briefly discuss a simple model for graphene and the novel way surface energy behaves in that system. For the off-lattice case I will introduce a rejection-based algorithm that offers the potential to greatly accelerate such simulations. This will be demonstrated by applying the method to the growth of two-species nanoclusters with a core-shell structure.

## **Arunima Singh**

### *A density-functional theory-based approach for aqueous stability of materials*

Aqueous media-based electrochemical processes such as water purification and electrocatalysis routinely operate devices at finite potentials and pH where materials stability is strikingly different from ambient conditions. In this talk I will describe our density-functional theory-based formalism [1] to assess the propensity of materials toward electrochemical stabilization, passivation, or corrosion in aqueous media. This formalism allows us to evaluate the relative Gibbs free energy of arbitrary materials with respect to Pourbaix stable species at any pH, voltage, temperature, and concentration of ions. Benchmarking against 20 stable as well as metastable materials reported in the literature and also our experimental investigation of metastable triclinic-FeVO<sub>4</sub>, we present quantitative estimates

for the relative Gibbs free energy and corresponding aqueous regimes where materials are most likely to be stable, form inert passivating films, or steadily corrode to aqueous species. The implementation of this formalism is freely available via the Materials Project github repository at <https://github.com/materialsproject/pymatgen>, allowing the programmatic determination of electrochemical stability of arbitrary materials, including the 69,000 materials available through the Materials Project Database.

I will discuss how this *ab initio* density-functional theory-based approach can be combined with molecular dynamics simulations to parametrize phenomenological models [2] to determine rate of corrosion, passivation film thickness as a function of time as well as the electronic properties of the passivated films.

[1] Singh, A.K., Zhou, L., Shinde, A., Suram, S.K., Montoya, J.H., Winston, D., Gregoire, J.M. and Persson, K.A., 2017. Electrochemical Stability of Metastable Materials. *Chemistry of Materials*, 29, 10159–10167 (2017).

[2] Macdonald, D. On the existence of our metals-based civilization. I. Phase-space analysis. *Journal of Electrochemical Society*, 153 (7), B213– B224 (2016).

### **Doaa Taha**

#### *Phase field crystal modeling of structures and dynamics of binary two-dimensional materials*

We introduce a binary phase field crystal (PFC) model to study various structures and dynamics of binary two-dimensional materials. Two topics will be discussed. The first topic is the use of the model to investigate the self-assembly of 2D binary colloidal structures with sublattice ordering. Several ordered phases and their coexistence states are investigated. We also identify experimentally observed structures and theoretically predict some new phases, along with their corresponding stability and phase diagrams. Phase transformation and grain nucleation and growth of these modulated/ordered phases are examined. The second topic is the parameterization of the PFC model for the study of hexagonal boron nitride monolayers. Structures, energies, and dynamics of both symmetrically and asymmetrically tilt grain boundaries are identified. Our results reproduce all types of dislocation cores found in previous experiments and first-principles calculations and predict new defect structures for various boundary misorientations, including 60° inversion domain boundaries. Finally, we identify a defect-mediated growth dynamic for inversion domains governed by the collective atomic migration and defect core transformation at grain boundaries and junctions, a process that is related to inversion symmetry breaking in binary lattices.

### **Gyula Toth**

#### *Hydrodynamic equations to the classical n-body problem: a quest for the viscosity*

One of the most robust principle of physics is undoubtedly the second law of thermodynamics, which states that macroscopic processes are irreversible. In the framework of statistical physics, the key step in proceeding from the BBGKY hierarchy to Boltzmann's H-theorem is the Hypothesis of Molecular Chaos: We assume, that the velocities of colliding particles are uncorrelated prior to the collision, and independent of position. We shall see, that even though the statistical physics based coarse graining procedure of the n-body problem indeed result in a viscous Navier-Stokes equation, exact (i.e., not probability-based) coarse graining methods can result only in inviscid (and therefore reversible) hydrodynamic equations for individual systems. The result is reasonable, when taking into account that Laplace's demon is present in the classical n-body dynamics. To resolve the problem, we propose a stochastic correction of the Hamiltonian equations, which, under the conservation of mass, momentum and energy, prescribes the coinstantaneous uncertainty of position and momentum, which therefore corresponds to information dissipation. A possible effect of this non-classical correction can be diffusive momentum transfer from long length scales to microscopic ones. In a broader context, the results suggest that the necessary condition for the second law of thermodynamics is quantum mechanical uncertainty, which is in agreement with recently published results of E. Hänggi and S. Wehner, *Nature Comm.* 4, 1670 (2013).

**Peter Voorhees***The phase field method: crystal structures and facets*

Phase field crystal (PFC) method allows the atomic scale motion and defect formation to be determined on diffusive timescales. A major challenge with the method is to devise free energy functions that can yield complicated crystal structures. We introduce a phase-field crystal model that creates an array of complex three- and two-dimensional crystal structures via a numerically tractable three-point correlation function. This approach successfully yields energetically stable simple cubic, diamond cubic, simple hexagonal, graphene layers, and CaF<sub>2</sub> crystals, as well as the particularly complex and technologically important perovskite crystal structure. Highly anisotropic interfaces play an important role in the development of material microstructure. We examine the capability of the PFC model to quantitatively describe faceted interfaces by coarse graining the PFC model to attain both its complex amplitude formulation, and its corresponding phase field limit. Using this formulation, we find that the model yields Wulff shapes with missing orientations, the transition to missing orientations, and facet formation. We demonstrate, in two dimensions, how the resultant model can be used to study the growth of crystals with varying degrees of anisotropy in the phase-field limit.

**Arthur F. Voter***Introduction to infrequent-event methods for materials and accelerated molecular dynamics methods*

Many important materials processes take place on time scales that far exceed the roughly one microsecond accessible to molecular dynamics simulation, making it difficult to develop a full microscopic understanding of material behavior. Typically, this long-time evolution is characterized by a succession of thermally activated infrequent events involving defects in the material. In this talk, I will present a brief introduction to this infrequent-event behavior and to some of the basic methods (transition state theory, kinetic Monte Carlo, and accelerated molecular dynamics) for exploiting this behavior to reach longer simulation times. Time permitting, I will also discuss some of our recent developments in accelerated molecular dynamics methods.

**David Wales***Exploring energy landscapes: molecules, nanodevices and condensed matter*

The potential energy landscape provides a conceptual and computational framework for investigating structure, dynamics and thermodynamics in atomic and molecular science. This talk will summarise new approaches for global optimisation, quantum dynamics, the thermodynamic properties of systems exhibiting broken ergodicity, and rare event dynamics. Applications will be presented that range from prediction and analysis of high-resolution spectra, to coarse-grained models and design principles for self-assembly of mesoscopic structures.

## Selected Publications:

D.J. Wales, *Curr. Op. Struct. Biol.*, 20, 3-10 (2010)

D.J. Wales, *J. Chem. Phys.*, 130, 204111 (2009)

B. Strodel and D.J. Wales, *Chem. Phys. Lett.*, 466, 105-115 (2008)

D.J. Wales and T.V. Bogdan, *J. Phys. Chem. B*, 110, 20765-20776 (2006)

D.J. Wales, *Int. Rev. Phys. Chem.*, 25, 237-282 (2006)

**Lei Zhang***A priori and a posteriori error estimates for multiscale coupling method*

I will talk about some recent progress on multiscale coupling methods for materials defects. We have derived a priori and a posteriori error estimates for atomistic/continuum (a/c) coupling with a unified analytical framework, and developed more accurate and efficient schemes based on those estimates. I will also talk about extensions to adaptive QM/MM coupling.