

Description of Research and Research Interests

To gather under a common *trait d'union* my so far brief career in physics feels somehow artificial, as I have touched different subjects with various techniques, from hard condensed matter, to granular materials, to statistical mechanics, and nonlinear physics, even to botany, while my interests now are extending to biophysics and DNA. Possibly a sign of dangerous eclecticism, or perhaps just a need for fun, my hopping between different themes finds its unity partially in the mathematical framework, partially at some unconscious level, and yet may be classified as covering two areas, broadly defined

1-Nanoscale Physics: I investigate electromechanical and statistical mechanical properties of different nanostructures, from mesoscopic materials like graphene or carbon and boron nitride nanotubes, and especially quasi-one-dimensional systems as nanowires, nanotubes, DNA strands, and also artificially frustrated two-dimensional metamaterials such as Artificial Spin Ice, which I have co-introduced. I employ a variety of techniques, often but not always based on some field theory approach and the analysis of the symmetries of the problem at hand.

2-Pattern Formation and Nonlinear Physics: I study in particular novel dynamics excitations in physical systems whose statics replicates the number theoretical patterns seen in biology. In this context I have introduced “dynamical phyllotaxis”.

My strategy in research is to strive for simple, result-oriented ideas, and to approach a problem from different perspectives, with a variety of methods, theoretically and often in collaboration with experimentalists (in fact publications in which I am not the first author are collaborations with experimentalists).

As an example of my work with experimentalists, in collaboration with Peter Schiffer and his group at Penn State, we introduced so-called Artificial Spin Ice [*Nature* **439** 303 (2006), *PRL* **101** 037205 (2008)], to study frustration in a system that can be imaged directly and engineered to demonstrate different physical properties. This work has generated substantial interest and is now pursued by many groups in USA (University of Maryland, Johns Hopkins), Europe (Imperial College, PSI), China, Brazil and Australia (see for example the recent dedicated Bragg-Stoner symposium at the University of Leeds in July 2010). Also, I have shown [*PRL* **98** 217203 (2007), *PRL* **105** 047205 (2010)] that the outcome of experiments on artificial spin ice—an athermal system—can be predicted very simply by an effective temperature, the first effective temperature to be based on a truly energetic and complex model. In another example of work with experimentalists, and of my interest in nanostructures, I have collaborated with Peter Eklund at Penn State (who very unfortunately has recently passed away) in explaining the emergence of a D-band in the Raman spectrum of Graphene as a signature of graphene folding [*J. Phys. Cond. Mat.* **22** 334205 (2010)] as well at explaining the distribution of doped electronic charge in multi-wall carbon nanotubes, in terms of a “nanocapacitor” [*PRL* **90**, 257403 (2003)].

I also work, alone or in collaboration with other theoreticians, at more analytical problems. For instance, independently and in a completely analytical work, I have introduced a symmetry based two-field formalism to describe the electromechanics of graphene and carbon nanotubes [*PRL* **99** 045501 (2007), *PRB* **80** 113406 (2009)], which predicts, with pen and paper, a wealth of phenomena inaccessible to the traditional continuum and provides a unified, analytically solvable framework for understanding and extending a previously disparate accumulation of

experimental and numerical results. In collaboration with Douglas Abraham from Oxford I have devised a thermodynamic formalism to study local failure in quasi-one-dimensional systems such as necking in nanowires, bubbles in DNA, or local collapses in nanotubes [*PRL* **102** 245504 (2009), *PRL* **104** 119902 (2010)] This model explains experimental results on nanowire growth as well as simulations of bubble opening in DNA. In a more interdisciplinary work, I introduced the idea of Dynamical Phyllotaxis: a novel set of excitations are revealed in systems of repulsive particles constrained in cylindrical geometries, whose statics is described by number theoretical laws of botanical Phyllotaxis: classical rotons and novel highly structured topological solitons [*PRL* **102** 186103 (2009), *PRE* **80** 026110 (2009), *PRE* **81** 046107 (2010)]. This work was recently featured in News and Views of Nature Materials, and in a column ("Farey Numbers and the Magnetic Cactus", Antony Phillips) for the American Mathematical Society.

My future work will concentrate mostly but not exclusively on

- 1) Artificially Frustrated metamaterials. This field, which I have initiated in collaboration with Schiffer and Samarth groups, is now growing at a fast pace. Many teams around the world are developing new experimental methods based on it, which could change our understanding of disordered matter. Already, the extension of thermodynamical formalism in these systems represents a successful application of a statistical treatment to a complex athermal system. Furthermore, artificial spin ice holds promises of future applications for, among other things, novel memory storage devices
- 2) Mechanics and thermodynamics of mesoscopic systems such as graphene, nanowires, nanotubes, and DNA strands. In my more theoretical and condensed matter oriented projects, I plan to study the statistical mechanics of the growth of nanowires, both in two and three dimensions. In particular, I am interested in nanowires grown in templates such as in nanopores which return tridimensional nanowires, and the growth in channels and associated issues of breakage due to lateral entropy gain. The latter can provide clues for experimentalists working at nanocircuits. I will also be working on the piezoelectricity of Boron Nitride nanotubes and boron-nitride-like structures. In particular, I am exploring the effect of symmetry breaking of the honeycomb lattice brought upon by the chiral vector for small tubes, and how that might allow for novel couplings between electric, magnetic and elastic fields.
- 3) A completely new set of projects pertains to my recent interest in the mechanics and thermodynamics of DNA and proteins. My interest in DNA developed from my work in quasi-one-dimensional systems and I am currently constructing models to describe its single-molecule mechanical behavior. At a preliminary level, I am able to predict, with pen and paper, many experimental results, including denaturation under unwinding, the transition to P-DNA under overwinding, and the anomalous overwinding under small stretch recently reported by Bustamante and others (Nature 2006). I am interested both in the biological applications and in the use of DNA as a nanomaterial. Mechanical properties of DNA are relevant for DNA's biological functions as it is well known that enzymes involved in replication exert elastic forces on the double helix, and in fact the kinetics of certain biological processes can be controlled by external load. Also, and perhaps more relevantly, the careful analysis of DNA mechanical and electromechanical properties could lead to faster and more efficient sequencing. But DNA holds a lot of promise also as a nanomaterial, since it can be manipulated as a single molecule. In particular I am interested in developing a DNA-based molecular motor that exploits the z-DNA to b-DNA transition (a switch based on a similar mechanism has already

been realized), via a propagation back and forth of a phyllotactic soliton along the double helix. The desired effect would be to chemically control the rotatory motion by acting on the solvent.

These three areas of investigation promises new fundamental insights and potential applications. Artificially frustrated metamaterials holds the promise of experimentally verifiable extensions of statistical mechanics, while being very relevant for memory storage devices. This new field, which we have invented, just had its first dedicated conference and it is now being developed in new directions by many groups around the world. Study of mesoscopic structures at the nanoscale, which started theoretically about twenty years ago, has been booming in terms of real implementations, with the latest Nobel prize being awarded for the realization of graphene sheets. Recently graphene sheets have been made in macroscopic size. The mechanical and electrical properties of DNA have been investigated experimentally for about fifteen years via single molecule manipulation, and while many experimental results await theoretical understanding, new DNA based nanomaterials are currently being proposed and realized. There is also an emerging trend in trying to exploit the mechanical and electrical properties of DNA to develop faster and cheaper ways of sequencing it (by controlled unzipping, by charge transport through a nanopore, and so on), and my modeling has potentials this area.