August 26

Isaac Alcón
Institut Català de Nanociència i Nanotecnologia, España

Title: Twisting between topological phases in 1D conjugated polymers

Abstract

In recent years it has become possible to tailor, with atomic precision, topologically protected states in carbon nanostructures like graphene nanoribbons[1] or 1D conjugated polymers (1DCPs).[2] Though different means have been proposed to tune trivial and non-trivial topological phases in such nanomaterials, such as hydrogenation[3] or electric fields,[4] aryl ring twist angles have not yet been considered. However, ring twisting has been shown to enable external control over electron pairing in 2D conjugated polymers via, for example, uniaxial strain.[5] Here, via accurate first principles density functional theory simulations, we demonstrate that aryl ring twist angles may indeed be used to transit from the trivial to non-trivial phases in 1DCPs made of triarylmethyl (TAM) units. Interestingly, we find that the quantum transition between the phases goes through an antiferromagnetic multiradical state displaying a finite bandgap. Thus, aside from establishing a connection between aryl ring twist angles and topology, we also demonstrate, for the first time in a carbon nanostructure, that the topological quantum phase transition may occur without bandgap closure, highlighting TAM 1DCPs as exotic topological nanomaterials.[6]

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Caio Lewenkopf
Universidade Federal Fluminense, Brazil

Title: Strongly disordered and amorphous topological insulators

Abstract

Topological materials are characterized by topological invariants whose evaluation usually relies on translational symmetry. As a consequence, the natural question that arises is: Can strongly disordered, non-crystalline, and amorphous display topological properties? Substantial theoretical work shows that this is indeed the case. After a brief review on the tools to characterize topological phases, I will discuss the most important advances in the research of strongly disordered and/or amorphous topological insulators, illustrating the main results using simple lattice models. Finally, I will present our ab initio studies that aim at proposing physical realizations of amorphous topological insulators.

August 27

Stephan Roche
(Institut Català de Nanociència i Nanotecnologia, España)

Title: Linear scaling quantum transport methodologies & applications to Topological Matter

Abstract

I will present the frame of efficient linear scaling transport methodologies (www.lsquant.org) which enable the simulation of realistic (three-dimensional) models of topological matter including the presence of disorder [1,2] and recently extended to other non-equilibrium regimes (hot electrons and energy dissipation).

I will illustrate the use of these approaches in various situations, focusing on spin transport properties in two-dimensional materials, topological insulators and van der Waals heterostructures. We will particularly review the initial claims of giant spin Hall effect in graphene-based devices and the upper limit that could be achieved by proximitized graphene with strong spin-orbit coupling materials. The combination of bulk-like approaches (Kubo formalism) and multiterminal transport methods (as for instance implemented within Kwant) will be shown essential to explore topological effects in complex disordered materials, and avoid ambiguous or misleading interpretations.

References
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Santiago Galván
(UNAM)

Title: Atomically Thin Current Pathways in Graphene through Kekulé-O Engineering

Abstract

We demonstrate that the current flow in graphene can be guided on atomically thin current pathways by the engineering of Kekulé-O distortions. A grain boundary in these distortions separates the system into topologically distinct regions and induces a ballistic domain-wall state. The state is independent of the orientation of the grain boundary with respect to the graphene sublattice and permits guiding the current on arbitrary paths. As the state is gapped, the current flow can be switched by electrostatic gates. Our findings are explained by a generalization of the Jackiw–Rebbi model, where the electrons behave in one region of the system as Fermions with an effective complex mass, making the device not only promising for technological applications but also a test-ground for concepts from high-energy physics. An atomic model supported by DFT calculations demonstrates that the system can be realized by decorating graphene with Ti atoms.

August 28

Parisa Majari
(Tecnológico de Monterrey)

Title: **Computational Investigations of Electronic Transport in 2D Materials**

Abstract

In the first part of our research, we studied the electronic properties and transport behaviors of monolayer and bilayer graphene under the influence of Rashba spin- orbit coupling. Using rigorous computational modeling, we have investigated the transmission coefficient of particles crossing potential barriers in these 2D systems, considering various free parameters to gain enhanced control over the transport characteristics. This understanding has led to insights that could potentially enable the development of novel transistor devices based on 2D materials. Building upon this work, we have further explored the electronic transport properties of few-layer graphene systems. Leveraging the Kwant software package, we have performed advanced simulations to study the transmission coefficient and current characteristics of particles interacting with potential barriers in these few-layer graphene structures.

Jesús Sánchez
(UNAM)

Title: **Electronic and transport properties of twisted bilayers".**

Abstract

"We investigate the electronic and transport properties of graphene twiste bilayers with a combination of molecular dynamics, tigh-binding models and the Green's function method. First, a nanoelectronic device made of twisted bilayer graphene (TBLG) is proposed to steer the direction of the current flow. The ballistic electron current, injected at one edge of the bottom layer, can be guided predominantly to one of the lateral edges of the top layer. The current is steered to the opposite lateral edge, if either the twist angle is reversed or the electrons are injected in the valence band instead of the conduction band, making it possible to control the current flow by electric gates. The observed steering angle exceeds well the twist angle and emerges for a broad range of experimentally accessible parameters and the steered current is valley polarized. We then move on to twisted bilayer graphene systems with a twist angle of $\theta \approx 1.696°$. We find two superlattice gaps in the energy spectrum of the bulk that are populated by edge-localized states in the case of nanoribbons. We demonstrate that the edge sates carry electronic current bidirectionally along the edges of a device with conductance values close to the conductance quantum. These states can be identified via non-local resistance measurements due to the fact that these states are localized only at certain edges of the system, depending on how the nanoribbon has been cut from the bulk. Technologically, our work is of relevance for nanoelectronic applications and will ramp the rising field of twistronics."

August 29

Jorge Lizárraga
(UNAM)

Title: **Electronic transport and anti-super-Klein tunneling in few-layer black phosphorous**

Abstract

This study examines the electronic transport properties of a multilayer phosphorene system using non-equilibrium Green's functions, considering interactions up to the 4th nearest neighbors. The findings demonstrate that anti-super Klein tunneling persists in this system. Additionally, the impact of oxidizing the top layer on electronic transport is investigated, revealing that the transport properties remain resilient despite this oxidation.

August 30

Stefan Bromley

Title: **From Molecular Radicals to 2D Quantum materials**

Abstract

A few years ago, we proposed using stable triarylmethyl radicals as novel open-shell building blocks for 2D covalent organic radical frameworks (2D CORFs) [1,2]. When forming a hexagonal lattice, we calculated that 2D hex-CORFs would exhibit antiferromagnetic (AF) ground states and would have energetically close lying closed-shell quinoidal and graphene-like semimetallic states [2]. Soon after this prediction, the first 2D hex-CORF was synthesised and was indeed found to show an AF state [3].
The AF state in 2D hex-CORFs is associated with a parent correlated Mott insulating phase in which unpaired spin-carrying electrons are localised on the radical nodes of the framework [2]. From this parent AF state, graphene-like semimetallic and closed-shell quinoidal/dimerised states should be accessible by modest out-of-plane compression [4] or in-plane strain [5], respectively. Recently, we have studied partial chemical substitution of the spin-carrying C centres in 2D hex-CORFs by B or N.
The resulting materials can be viewed as 2D extensions of neutral mixed valence compounds and exhibit emergent spin-frustrated triangular lattices which have the potential to host a range of exotic quantum states (e.g. superconductivity, spin-liquid, novel magnetic ordering) [6]. Overall, our findings establish 2D hex-CORFs as a new class of 2D multifunctional quantum materials that can be tuned by stress/strain/substitution for potential future technological applications.

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Tathagata Kar

Title: Multidimensional carbon materials for electrochemical energy storage and conversion

Abstract

Multi-dimensional carbon materials feature in a myriad of energy-based applications ranging from electrocatalysts to supercapacitors and sensors to batteries. This is primarily because the environment-friendly, cost-effective, and well-conducting carbon-based materials possess excellent characteristics towards efficient electrochemical energy conversion and storage. Studies suggest that the electrochemistry of carbon can be significantly altered (or enhanced) by fine-tuning its physical structure and surface modification. Herein, the interesting electrochemistry of a wide range of porous and laminar carbon structures towards electrochemical energy storage and conversion is discussed.

September 03

Mesías Orozco-Ic

Title:Magnetic response properties in molecules as a way to diagnose electron delocalization

Abstract

Magnetic fields induce current densities in all atoms and molecules in response to the external field. In cyclic molecules, the induced current density flows, creating ring currents, which in turn generate an induced magnetic field. Depending on the direction of the current, this induced field points either parallel or antiparallel to the external magnetic field. This molecular magnetic response to an external magnetic field is of great interest in molecular chemistry and physics because it functions as a molecular fingerprint. In other words, it is unique to each system and depends on the electronic nature of the molecule. These magnetic responses are obtained using joint techniques from electromagnetism and quantum mechanics, providing a solid rationale for complex concepts such as aromaticity and chemical bonding through the quantification of physical properties induced in both planar and three-dimensional molecules.

Aromaticity, in particular, is a fundamental concept in chemistry that helps explain a set of properties exhibited by certain cyclic compounds, such as high energetic stability, remarkable symmetry, low reactivity, and characteristic magnetic properties. The calculation of molecular magnetic response is essentially the quantum mechanical theory behind nuclear magnetic resonance (NMR) experiments. Therefore, there is a bridge between experiment and theory, which explains why magnetic criteria have gained popularity and success in the scientific community when quantifying electronic delocalization, allowing the design of smart materials based on (anti)aromatic compounds whose properties can be controlled through their interaction with electromagnetic fields.

However, determining the degree of aromaticity through the analysis of magnetic response is not a trivial task and often requires the simultaneous study of various magnetic criteria. In this work, the magnetic response of molecules was analyzed in depth within the framework of nuclear magnetic shielding theory, considering the warnings and limitations corresponding to the use of magnetic criteria to determine the degree of electronic delocalization. The role of molecular geometry, topology, curvature, core electron contributions, and relativistic and spin-orbit corrections to molecular magnetic response is investigated using density functional theory. The analysis focuses on the calculation and visualization of induced magnetic fields and induced current densities and their relationship to one another.

Our results establish the systematic and rational study of the magnetic response of small and nanometric-scale molecular systems, leading to the design of new smart materials based on systems where magnetic properties and their relationship to aromaticity play a key role.

Rosa Di Felice

Quantum simulations of fermionic and spin Hamiltonians

Despite huge efforts and significant progress in algorithmic development and error reduction techniques, there is not yet evidence of quantum performance/advantage in solving useful computational problems in chemistry and materials science. But why should we use quantum computers?

In this presentation, I will attempt conceptual answers to this question and show preliminary data towards these answers.

More specifically, I will:

1. Identify the bottlenecks of classical algorithms for the solution of the Schrödinger equation of molecules and materials from first principles, which is where quantum algorithms can be grafted; in this context, I will focus on examples of molecules with strong electronic correlations and show the current level of feasibility of quantum calculations on a prototype system;

2. Design a multi-disciplinary protocol for the computational solution of groundbreaking applications, which goes from the identification of domain relevant applications, to the distillation of mathematical problems, to the formulation of quantum algorithms and implementation in quantum software/hardware; in this context, I will use the electron transfer problem as an example.

September 05

Yael Hernández

Emulation of non-abelian fields in tight-binding lattices.

Abstract

In this work the incorporation of non abelian fields SU(N) on the tight-binding approximation is presented by the introduction of the minimal coupling for discrete systems. The U(1) field emulations are obtained by the use of chains of rotating dimers. The Hamiltonian can be written in terms of the symmetric and antisymmetric states of each dimer of the chain which allows us to obtain a Hamiltonian with two decoupled blocks that correspond to two U(1) field theories. The Hofstadter butterfly emerges in the antisymmetric band when the distance between centers of the dimers vary. In the symmetric band we observe the spectrum of the Harper Hamiltonian with $\Lambda \neq 6$.

Humberto Saint-Martín

Exploring the Dynamic Coordination Sphere of Lanthanide Aqua Ions: Insights from r2SCAN-3c Composite-DFT Born-Oppenheimer Molecular Dynamics Studies.

Abstract

Born-Oppenheimer molecular dynamics (BOMD) simulations are done to investigate the structure and dynamics of the first hydration shells of five trivalent lanthanide ions (Ln3+) at room temperature that are relevant in various environments, including the bulk aqueous solution. A cluster microsolvation approach was employed to address the interaction of Ln3+ ions (La, Nd, Gd, Er, and Lu) with up to 27 explicit water molecules. Electronic structure calculations were performed using the composite r2SCAN-3c method. The results demonstrate that this method offers an excellent balance between precision and computational efficiency. Specifically, it accurately predicts average Ln-O distances (MAE = 0.02 ˚A) of the first hydration sphere and preferredcoordination numbers (CN) for the different lanthanide cations as compared to reported data in bulk. Highly dynamic first hydration shells for the examined Ln3+ ions were found, with noticeable and rapid rearrangements in their coordination geometries, some of which can be recognized as the Tricapped Trigonal Prism (TTP) and the Capped Square Antiprism (CSAP) for CN = 9, and as the Square Antiprism (SAP), the Bicapped Trigonal Prism (BTP), as well as the Trigonal Dodecahedron (DDH) for CN = 8. However, ca. 70% of the nonacoordinated configurations did not meet the criteria of TTP or CSAP structures. For CN = 8, the percentage of configurations that could not be assigned to either SAP, BTP or DDH was lower, around 30%. The theoretical EXAFS spectra obtained from the BOMD simulations are in good agreement with the experimental data and confirm that model microsolvated environments accurately represent the near solvation structure of these trivalent rare-earth ions. Moreover, this shows that the faster dynamics of the first hydration shell can be studied separately from that of water exchange in the bulk aqueous solution.

September 06

Dr. Rafael Méndez

Title: Coupled-resonator phononic systems: emulating spectra of atomic and condensed matter physics”

Abstract

Recent results in the vibrations of coupled-resonator phononic waveguides are presented. These waveguides are composed of resonators coupled through finite phononic crystals called couplers. When a normal-mode frequency of the resonator falls within the coupler bandgap, the waveguide modes get trapped in the resonators. These modes connect to neighbor resonators through evanescent waves and obey an analog of the tight-binding model of condensed-matter physics. Applications in linear and aromatic molecules are presented. A broad discussion about the methods used will be given.