# TT 27: Focus Session: Designer Quantum Systems I (joint session O/TT)

Toy models are simplistic theoretical constructs, meant to capture the basic principles of complex phenomena observed in experiment. Recent amazing advances in condensed matter physics have enabled the reverse, namely the realization of basic theoretical models in well-controlled artificial experimental systems. Such solid state or molecular realizations of models allow us to tune their parameters, thus they may be termed designer quantum systems and can substantially deepen our understanding. Some talks in this session explore the insights offered by the already famous designer quantum systems; others propose or even report new quantum simulators. Moreover, these designer systems are not limited to single-particle physics but extend to many-body phenomena, such as superconducting correlations.

Organizers: Magdalena Marganska and Jascha Repp (University of Regensburg).

Time: Tuesday 10:30–12:45 Location: H15

**Invited Talk** TT 27.1 Tue 10:30 H15

**Imaging Electronic Correlations in Twisted Bilayer Graphene** — •Stevan Nadj-Perge — California Institute of Technology, Pasadena, CA, USA

Twisted bilayer graphene with a twist angle close to 1° features isolated flat electronic bands that form a strongly correlated electronic system. Here we investigate properties of this system by probing local tunneling density of states using scanning tunneling microscopy and spectroscopy. We show that the flat bands get deformed when they are aligned with the Fermi level using electrostatic gating. Careful characterization of the bands allows us to estimate energy scale of electron-electron interactions. Our results provide basis for microscopic understanding of correlated quantum phases in small angle twisted bilayer graphene.

**Invited Talk** TT 27.2 Tue 11:00 H15

**Designing Electronic Quantum Matter: Fabrication and Characterization with Atomic Scale Precision** — •Ingmar Swart — Debye Institute for Nanomaterials Science

In a visionary colloquium nearly sixty years ago, Richard Feynman proposed to study complex and elusive quantum systems using more controllable analogues, an approach known as quantum simulation [later published, 1]. Although quantum simulation based on ultracold atoms in optical lattices, nanophotonic systems, trapped ions and superconducting circuits has been very fruitful, electronic quantum simulators have been lacking behind [2].

In this talk, I will demonstrate that electron gases on well-defined metal surfaces form an excellent platform for quantum simulation. By patterning the surface with atomic scale precision using a scanning tunneling microscope, the electrons can be corralled into artificial lattices of nearly any geometry. The same microscope can then be used to measure the local density of states at all positions of interest and to probe the spatial extend and shape of the wave functions. I will show several examples of how we exploit the tunability of this platform. Particular emphasis will be given to our recent efforts to create and study electronic higher-order topological insulators.

References: 1. Richard P. Feynman, International Journal of Theoretical Physics, 21, 467 (1982). 2. Nature Physics Insight on Quantum Simulation, Volume 8 (2012).

TT 27.3 Tue 11:30 H15

**Characterisation of pure s- and p-orbital bands in electronic honeycomb lattices** — •Thomas Gardenier[1], Jette van den Broeke[2], Ingmar Swart[1], Cristiane Morais Smith[2], and Daniel Vanmaekelbergh[1] — [1]Debye Institute for Nanomaterials Science, Utrecht, The Netherlands — [2]Institute for Theoretical Physics, Utrecht, The Netherlands

Honeycomb systems have generated much interest in experimental and theoretical physics due to their interesting band structures. The architypical example of a honeycomb lattice is graphene. The electronic structure of graphene close to the Fermi level can be understood by only considering C 2pz orbitals. Bands due to coupling of sp2 hybrid orbitals are either much higher or lower in energy. It has been shown that in the absence of hybridisation, the band structure of honeycomb lattices features a topologically non-trivial flat band, as well as Dirac cones formed by px and py orbitals.

We patterned a Cu(111) surface with CO molecules to confine the surface state electrons into a honeycomb geometry. By careful tuning of the lattice parameters, we created a honeycomb lattice where s- and p-orbital bands are separated. Scanning tunneling spectroscopy and wavefunction mapping are used to determine the band structure and visualise the electron densities. The results are complemented by theoretical muffin-tin and tight-binding calculations.

TT 27.4 Tue 11:45 H15

**Constructing a Topological Insulator Atom-by-Atom** — •Saoirsé Freeney — Condensed Matter and Interfaces, Princetonplein 1, 3584 CC Utrecht, The Netherlands

In a honeycomb lattice with alternating hopping strengths (Kekulé lattice), a gap in the energy dispersion is opened. Depending on the ratio of hopping parameters and the shape of the boundary, the band structure is either topologically trivial or non-trivial. Using scanning tunnelling microscopy, we realize Kekulé lattices through the coupling of artificial atoms, created by the careful arrangement of electron scatterers (carbon monoxide molecules) on a 2D electron gas (Cu(111) surface state). The electronic properties were probed using scanning tunnelling spectroscopy and differential conductance mapping. We show that the topologically non-trivial lattice features a robust edge state whereas the trivial equivalent does not. The experimental outcomes align well with results from tight binding and muffin tin calculations.

TT 27.5 Tue 12:00 H15

**Eu-doped NaI scintillators: Point defects and $EuI_2$ sheets.** — •Martin Setvin[1], Manuel Ulreich[1], Igor Sokolovic[1], Michele Reticcioli[3], Lynn Boatner[2], Flora Poelzleitner[1], Cesare Franchini[3], Michael Schmid[1], and Ulrike Diebold[1] — [1]Institute of Applied Physics, TU Wien, Vienna, 1040, Austria — [2]Materials Science and Technology Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee, 37831, USA — [3]Faculty of Physics and Center for Computational Materials Science, University of Vienna, Vienna, Austria

Activator impurities and their distribution in the host lattice play a key role in scintillation phenomena. A combination of cross-sectional noncontact atomic force microscopy (nc-AFM) and X-ray photoelectron spectroscopy (XPS) was used to study the distribution of $Eu^{2+}$ dopants in a NaI scintillator activated by 3% of $EuI_2$. Two types of precipitate structures were identified. First, a single-sheet of $EuI_2$ layered precipitate is a favoured configuration at the surface. Second, precipitates with a cubic crystal structure and a size below 4 nm were found in the bulk material. A surprisingly low concentration of point defects was detected in all of the investigated samples. The relation between the atomic structure and scintillation will be discussed.

The work was supported by the FWF Wittgenstein Prize Z-250.

TT 27.6 Tue 12:15 H15

**Machine learning the 3D shape of non-planar molecules from AFM images** — •Prokop Hapala[1], Fedor Utirev[1], Niko Oinonen[1], Ondřej Krejčí[1], Filippo Federici Canova[1], Benjamin Alldritt[1], Juho Kannala[2], Peter Liljeroth[1], and Adam Foster[1] — [1]Department of Applied Physics, Aalto University — [2]Department of Computer Science, Aalto University

In recent decade Atomic Force Microscopy with tip functionalized by carbon monoxide (CO) provided unique tool to experimentally image sub-molecular details of individual organic molecules [1]. Yet up to now most experiments are limited to flat aromatic molecules, due to difficulties with interpretation of highly distorted images originating from non-planer molecules due to mechanical relaxation of tip or sample. These problems can be partially overcome using a simple mechanical model [2] which can reproduce those distortions, therefore simulate AFM images for given molecular structure. Testing many possible

candidate structures is, however, laborious. Instead we attempt to develop automatic tool to conduct inverse task - i.e. to recover molecular structure from given set of AFM images. Preliminary results suggests that convolutional neural network (CNN) [3] trained on simulated AFM images can learn this inverse mapping rather easily. Yet application of the method on real experimental data, and identification of atomic species remains to be a challenge. [1] Gross, L., et al., Science, 325(5944), 1110-1114 (2009). [2] Lecun, Y., et al., Proceedings of the IEEE, 86(11), 2278-2324 (1998). [3] Hapala, et al. PRB, 90(8), 085421 (2014).

TT 27.7 Tue 12:30 H15

**Spectral Properties of the Herringbone lattice** — M. A. Jimenez Herrera[1], O. Dutta[2], A. Iniguez[3], G. Giedke[2,4], and •D. Bercioux[2,4] — [1]Centro de Física de Materiales (CFM-MPC) Centro Mixto CSIC-UPV/EHU, E-20018 Donostia-San Sebastián, Spain — [2]Donostia International Physics Center (DIPC), Paseo Manuel de Lardizbal 4, E-20018 San Sebastián, Spain — [3]University of the Basque Country, UPV/EHU, Bilbao, Spain — [4]IKERBASQUE, Basque Foundation of Science, 48011 Bilbao, Spain

We investigate the spectral properties of a two-dimensional lattice system described by a non-symmorphic symmetry; specifically, we look at the herringbone lattice that is characterised by two glide symmetries. We model the system via a tight-binding model with horizontal and vertical hopping terms. We evaluate the spectrum of the system in the presence of a perpendicular magnetic field: we show how the Hofstadter's butterfly presents characteristics inherited by the honeycomb and square lattice butterflies. Furthermore, we investigate the appearance of edge states in the system when dimerizing the hopping parameters on the horizontal and vertical direction. We analyse the topological properties of these bands in a similar way to the analysis presented for the case of a symmorphic lattice [1]. Finally, we present a possible implementation in terms of CO atoms placed on the top of a Cu(111) surface [2].

[1] F. Liu, & K. Wakabayashi Phys. Rev. Lett. **118**, 076803 (2017). [2] K. K. Gomes, W. Mar, W. Ko, F. Guinea, & H. C. Manoharan Nature, **483**, 306 (2012).