

O 36: Focus Session: Designer Quantum Systems II (joint session O/TT)

Time: Tuesday 14:00–15:45

Location: H15

Invited Talk

O 36.1 Tue 14:00 H15

Topological quantum phases in atomically precise graphene nanoribbons — ●OLIVER GRÖNING¹, SHIYONG WANG², QIANG SUN¹, AKIMITSU NARITA³, MÜLLEN KLAUS³, PASCAL RUFFIEUX¹, and ROMAN FASEL¹ — ¹Empa Materials Science and Technology, Dübendorf, Switzerland — ²School of Physics and Astronomy, Shanghai Jiao Tong University, Shanghai, China — ³Max Planck Institute for Polymer Research, Mainz, Germany

Topological materials have attracted great interest in solid state physics due to their ability to support robust, yet exotic quantum states at their boundaries or interfaces such as spin-momentum locked transport channels or Majorana fermions. Very recently, it has been found theoretically by Louie et al., that localized zero energy modes can be obtained at the junctions of topologically dissimilar graphene nanoribbons (GNR). We have experimentally realized such GNR junctions using on-surface synthesis, i.e. by the polymerization of molecular precursors rationally designed to yield the desired final GNR on single crystal surfaces. By creating well defined periodic sequences of these topological electronic modes, one-dimensional electronic bands can be created, which are described by the Su-Schrieffer-Heeger (SSH) Hamiltonian representing the dimerized atomic chain. By manipulating the intra- and inter-cell coupling strength we could further create SSH analogs with different winding number and therefore topological class. The topological class distinction is evidenced by presence, respectively absence of zero energy end states at the termini of the corresponding GNR or their junctions to structurally dissimilar GNRs.

Invited Talk

O 36.2 Tue 14:30 H15

Electronic properties of twisted graphene layers: bands, interactions and superconductivity. — ●FRANCISCO GUINEA — Imdea Nanscience, Faraday , 28049 Madrid, Spain — School of Physics and Astronomy, University of Manchester, Oxford Road, Manchester M13 9PL, UK

Twisted graphene bilayers show an unusual band structure, with very narrow bands. In these bands, states with different momenta show significant variations in their charge density. A change in the number of carriers leads to inhomogeneous charge distributions, which, in turn, modify significantly the shape of the bands. This effect can be described in terms of emergent assisted hopping interactions. These couplings tend to favor superconductivity.

O 36.3 Tue 15:00 H15

Symmetry breaking in Molecular Artificial Graphene — ●LINGHAO YAN^{1,2}, MUQING HUA², QIUSHI ZHANG², Tsz UE NGAI², ZESHENG GUO², Tsz CHUN WU², TONG WANG², and NIAN LIN² — ¹Aalto University, Finland — ²The Hong Kong University of Science and Technology, Hong Kong, China

Artificially-assembled molecular lattices on metal surfaces, known as molecular designers (Nature 483, 306, 2012), have been used as simulators to explore exciting physics that are extremely challenging to access in real materials. For example, gauge field, edge states and flat band are demonstrated in artificial graphene, graphene nanoribbons, and Lieb lattice. In this work, we exploit the unique tunability of the molecular designers to break the symmetry of Dirac quasiparticles. The importance of symmetry breaking in graphene for applications has been widely recognized. Several schemes have been proposed, including breaking sublattice symmetry and applying uniaxial strain. Here we report the realization of both of these schemes by design-

ing isotropic molecular potentials and isotropic lattices, respectively. The spatially-resolved local density of states acquired using scanning tunneling spectroscopy confirm that in both cases the local density of states undergo characteristic changes.

O 36.4 Tue 15:15 H15

On-Surface Synthesis and Characterization of Cycloarenes: a C108 Graphene Quantum Ring — ●QITANG FAN¹, DANIEL MARTIN JIMENEZ², SIMON WERNER¹, DANIEL EBELING², ANDRÉ SCHIRMEISEN², JÖRG SUNDERMEYER¹, WOLFGANG HIERINGER³, and J. MICHAEL GOTTFRIED¹ — ¹Fachbereich Chemie, Philipps-Universität Marburg, Germany — ²Institute of Applied Physics (IAP), Justus Liebig University Gießen, Germany — ³Lehrstuhl für Theoretische Chemie, Universität Erlangen-Nürnberg, Germany

Cycloarenes, such as kekulene, are a unique class of polycyclic aromatic hydrocarbons (PAHs). They enclose a cavity by circularly annulated benzene rings. In a modern view, they can thus be considered as nanorings cut-out from graphene with atomic precision. These graphene rings could serve as useful model quantum materials for the exploration of geometry-dependent electronic properties of nanographenes, e.g., the Aharonov-Bohm effect in graphene quantum rings. However, the synthesis and characterization of cycloarenes with more than one band of benzene rings is still challenging due to their special ring-shaped geometry and low solubility. Here, we employed the high-dilution principle both on a metal surface and in solution to synthesize a novel hexagonal cycloarene with two bands of annulated benzene rings, containing 108 sp² carbons, by hierarchical Ullmann coupling and cyclodehydrogenation reaction of dibrominated aromatic precursors. The structure and properties of this C108 cycloarene molecule has been unambiguously clarified by various techniques including STM/STS, nc-AFM, UV-vis spectroscopy, and DFT calculations.

O 36.5 Tue 15:30 H15

Nonlinear optical Hall effect in BC₂N — ●JULEN IBAÑEZ-AZPIROZ¹, IVO SOUZA^{1,2}, and FERNANDO DE JUAN^{2,3} — ¹Materials Physics Center, CSIC-UPV/EHU, 20018 Donostia-San Sebastián, Spain — ²Ikerbasque Foundation, 48013 Bilbao, Spain — ³Donostia International Physics Center (DIPC), 20018 Donostia, Spain

The bulk photovoltaic effect is a nonlinear optical response that yields a net photocurrent in noncentrosymmetric crystals. Its interband contribution under linearly polarized light, known as the *shift current*, involves a subtle Berry-phase-like quantity that makes this effect very sensitive to wavefunction properties. Here we show that the relative parity of valence and conduction bands under mirror reflection determines whether the shift current flows parallel or perpendicular to the applied electric field. The former situation is realized in GeS and similar monolayers [1,2] while the later, which corresponds to a nonlinear optical Hall effect, is far less common. Based on a recently developed *ab-initio* method [3], we show that this novel effect is realized in layer-structured graphitic BC₂N. Furthermore, our calculations reveal an enhanced shift-current absorption in the visible range, which makes BC₂N a prime candidate for future experimental studies.

[1] A. Cook, B. M. Fregoso, F. de Juan et. al., Nat. Commun. **8**, 14176 (2017).

[2] T. Rangel, B. M. Fregoso, B. S. Mendoza et. al., Phys. Rev. Lett. **119**, 067402 (2017).

[3] J. Ibañez-Azpiroz, S. S. Tsirkin and I. Souza, Phys. Rev. B **97**, 245143 (2018)