

RTG 2861 “Planar Carbon Lattices” Joint On-site Meeting in Dresden, April 18-19, 2024

Location: [TU Dresden, Mommsenstraße 13/15, Festsaal Dülferstraße](#)

TUD Campus Navigator: <https://navigator.tu-dresden.de/etplan/m13/01/raum/156101.0400>

Meeting program

Thursday, 18.04.2024, in Festsaal Dülferstraße (Mommsenstraße 13/15)

12:30 - 13:30 *Joint lunch and welcome coffee*

13:30 - 13:35 Opening remarks

13:35 - 14:05 Progress report **Majid Shaker**, Project A5, FAU,
Talk title: “Tetraphenyltransdibenzoporphyrins on Cu(111)”

14:05 - 14:35 Progress report **Anjana Aravind**, Project C1, TUD

14:35 - 15:40 Subgroup meetings of D.R. + PI supervisor + PI co-supervisor + collaboration partner available on-site, and online if possible;

- Feedback on annual written reports;
- Planning of lab-rotations/ research visits
- Individual discussions with the guest speaker

15:40 - 16:00 *Coffee break*

16:00 - 17:00 Guest talk by **Dr. Deborah Prezzi** (CNR-NANO, Modena, Italy),
Talk title: “Graphene nanoribbons for optoelectronic applications: insights from ab initio simulations”

18:30 - 20:30 Joint dinner at [Da Michele](#) (Louisenstraße 33, 01099 Dresden)

Friday, 19.04.2024, in Festsaal Dülferstraße (Mommsenstraße 13/15)

09:30 - 11:00 PI-meeting (PIs only)

11:00 - 11:30 *Coffee break*

11:30 - 12:00 Progress report **Boris Borisov**, Project A2, TUD

12:00 - 12:30 Remaining discussions & Closing remarks

12:30 - 13:30 *Joint lunch and departure*

RTG-PCL guest talk | April 18, 2024 | 16:00 | [Dülfersaal](#) and online

Graphene nanoribbons for optoelectronic applications: insights from ab initio simulations

Dr. Deborah Prezzi

S3 Center, Nanoscience Institute of the National Research Council (CNR-NANO), via Campi 213/a, I-41125 Modena, Italy

The bottom-up synthesis of graphene nanoribbons (GNRs) has become a consolidated route for exploring their size and width-dependent properties in view of graphene-based nano- and optoelectronic applications. Meanwhile, the rise of other 2D materials has opened new possibilities to investigate novel phenomena and design nanostructures with new functionalities.

Exploring the predictive power of ab initio simulations beyond mean field, I will discuss the optical response of atomically precise GNRs [1, 2] and their perspective for device applications. The possibilities connected to further modifications to the GNR structure, including edge functionalization [3] and synthesis of heterostructures [4] will be also discussed. The GNR properties will be compared with those predicted for nanoribbons based on different 2D materials, e.g. MoS₂ NRs [5].

References:

- [1] Bright Electroluminescence from Single Graphene Nanoribbon Junctions; Chong, M.C., Afshar-Imani, N., Scheurer, F., Cardoso, C., Ferretti, A., Prezzi, D., Schull, G.; *Nano Letters* **18**, 175-181 (2018)
- [2] Exciton-dominated optical response of ultra-narrow graphene nanoribbons; Denk, R., Hohage, M., Zeppenfeld, P., Cai, J., Pignedoli, C.A., Söde, H., Fasel, R., Feng, X., Müllen, K., Wang, S., Prezzi, D., Ferretti, A., Ruini, A., Molinari, E., Ruffieux, P.; *Nature Commun.* **5**, 4253 (2014)
- [3] Bandgap Engineering of Graphene Nanoribbons by Control over Structural Distortion; Hu, Y., Xie, P., De Corato, M., Ruini, A., Zhao, S., Meggendorfer, F., Straasø, L.A., Rondin, L., Simon, P., Li, J., Finley, J.J., Hansen, M.R., Lauret, J.-S., Molinari, E., Feng, X., Barth, J.V., Palma, C.-A., Prezzi, D., Müllen, K., Narita, A.; *JACS* **140**, 7803-7809 (2018); Band structure modulation by methoxy-functionalization of graphene nanoribbons; Götz A., Wang X.Y., Ruini A., Zheng W., Soltani P., Graf R., Tries A., Li J., Palma C.A., Molinari E., Hansen M.R., Wang H.I., Prezzi D., Müllen K., Narita A.; *J Mater Chem C* **10**, 4173-4181 (2022)
- [4] L. Adamska, M. Bonacci, D. Varsano, D. Prezzi, preprint (2023)
- [5] *Intrinsic edge excitons in two-dimensional MoS₂*; D'Amico, P., Gibertini, M., Prezzi, D., Varsano, D., Ferretti, A., Marzari, N., Molinari, E.; *Phys. Rev. B* **101**, 161410 (2020)