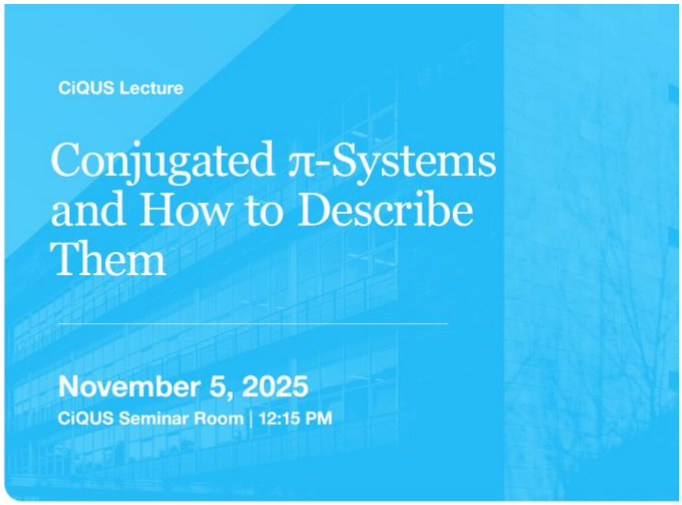
Dr. Igor Roncevic
University of Manchester



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Abstract

This talk will discuss the electronic structure of various π-conjugated systems in terms of simple (tight-binding) models. We will explore the relationship between aromaticity, coherence, and electronic structure, using cyclocarbons, annulenes, and porphyrin nanorings as examples.

Cyclo[*n*]carbons (Fig. 1a) are loops of *n* carbon atoms. Recent advances in scanning probe microscopy (SPM) have enabled the on-surface synthesis and characterisation of these unusual molecular carbon allotropes, which have long served as a playground for theoretical approaches.[1,2] We will compare SPM resonance images with high-level *ab initio* calculations, showing that the electronic structure of cyclocarbons can be captured by a particle-on-a-ring model.

Conjugated porphyrin nanostructures (Fig. 1b) display remarkable properties such as quantum interference and length-independent conductance, which make them excellent candidates for molecular electronics.[3] These properties stem from the coherent delocalisation of the wavefunction through the whole molecule, which becomes weaker as the molecule become larger. By analysing the ways in which π-systems can distort, we will estimate the maximum size at which edge-fused porphyrin nanorings (Fig. 1b) can still be expected to exhibit quantum behaviour.[4,5]

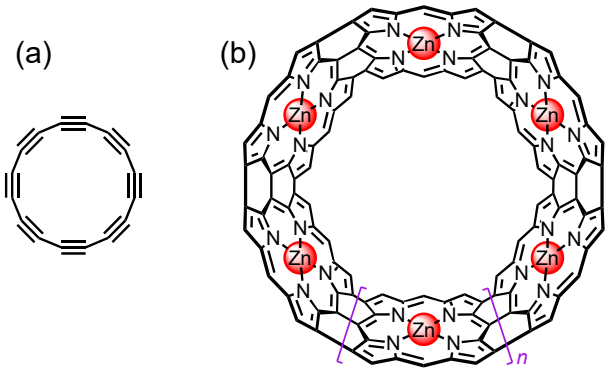

Fig. 1. *(a) Cyclo[16]carbon. (b) Edge-fused porphyrin nanoring.*

References

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[2] F. Albrecht, I. Rončević, Y. Gao, F. Paschke et al. *Science* **2024**, *384*, 677.
[3] J.-R. Den et al. *J. Am. Chem. Soc.* **2024**, *146*, 3651.
[4] M. Vitek et al. *ACS Nano* **2024**, 19, 1405.
[5] A. Rubio et al. *Science* **2025**, accepted, DOI: 10.26434/chemrxiv-2025-xxzl1

Biosketch

Igor Roncevic finished his PhD at the University of Zagreb in Croatia. He held a Czech Academy of Sciences-funded postdoctoral fellowship (2019–2021) with Josef Michl, staying in both Prague (Czechia) and Boulder (Colorado, US). In 2022 he was awarded a Marie Curie Felloship with Harry Anderson in Oxford, and in 2024 he started an independent research group at the University of Manchester.

In 2025, Igor and Iago Pozo were awarded a Royal Society of Chemistry research collaboration grant, which is funding this visit. Igor's main interest is in the electronic structure, aromaticity, and magnetism of π-conjugated systems.