Poster

Molecular Mosaics Discovery and Electron Crystallography

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Quantum materials exhibit exotic phenomena arising from the intricate interplay between electronic, magnetic, and lattice degrees of freedom. Virtually all quantum materials are inorganic in nature and synthesized under conditions that provide nothing but thermodynamic control as a synthetic handle. Molecular chemistry offers the tools for addressing contemporary problems in quantum materials discovery, enabling the rational design, synthesis, characterization, and understanding of novel materials. Metal-ligand assemblies with variable or hardly separable valences ("non-innocence") are pervasive in molecular coordination chemistry and host the possibility to tame strong electron-electron correlations in extended networks, thereby representing a realistic strategy to challenge current state-of-the-art in quantum materials discovery. The use of well-defined metal ion "building blocks" with predictable bonding characteristics as nodes, in conjunction with rigid molecular linkers, provides a novel strategy to synthetically tailor materials' tessellations. In the lecture I will discuss the group's recent findings in the quest for genuinely new symmetries and properties in metal-organic framework materials and showcase how the use of novel 3D electron diffraction methods applied in our laboratory will accelerate materials discovery, broadly defined.

[1] M. Dunstan, A. Manvell, N. Yutronkie, F. Aribot, J. Bendix, A. Rogalev, K. S. Pedersen, Nature Chemistry 2024, DOI: 10.1038/s41557-023-01422-8

[2] X. Liu, J. N. McPherson, C. E. Andersen, M. S. B. Jørgensen, R. W. Larsen, N. J. Yutronkie, F. Wilhelm, A. Rogalev, M. Gimenéz-Marqués, G. Mínguez Espallargas, C. R. Göb, K. S. Pedersen, Nature Commununications 2024, 15, 1177.

[3] P. Perlepe, I. Oyarzabal, L. Voigt, M. Kubus, D. N. Woodruff, S. E. Reyes-Lillo, M. L. Aubrey, Ph. Négrier, M. Rouzières, F. Wilhelm, A. Rogalev, J. B. Neaton, J. R. Long, C. Mathonière, B. Vignolle, K. S. Pedersen, R. Clérac. Nature Communications 2022, 13, 5766

[4] H. Chen, L. Voigt, M. Kubus, D. Mihrin, S. Mossin, R. W. Larsen, S. Kegnæs, S. Piligkos, K. S. Pedersen. Journal of the American Chemical Society 2021, 143, 14041.