

**Titre : "Synthesis of Novel Quantum Materials with Targeted Electronic Properties"**

1. **Organisateurs (avec affiliation, usuellement 2 ou 3 personnes)** : Andrea Gauzzi, Sorbonne Université, Paris and Sylvie Hébert, CRISMAT-ENSICAEN, Caen
2. **Parrainage ou lien avec des sociétés savantes, des GDR ou autres structures** : GDR Meeticc, GDR OXYFUN, GDR HOWDI, GIS Thermoélectricité
3. **Résumé de la thématique du minicolloque**

During recent years, the new capabilities offered by data mining, artificial intelligence and *ab initio* calculations have enabled the effective design and synthesis of materials with specific physical and functional properties. This has led to the prediction and, in some cases, to the experimental discovery of novel compounds, such as topological materials or superconductors, or to a comprehensive explanation of the remarkable properties of exotic phases, such as superconducting hydrides, and of promising functional materials, e.g. photonic crystals, thermoelectrics, magnetoelectrics and multiferroics.

These promising results suggest a powerful research direction combining theoretical predictions, data mining, artificial intelligence and advanced methods enabling the synthesis of metastable phases in both bulk and nanostructured or thin-film form and the optimisation of targeted properties.

The goal of the proposed workshop is to present recent advances in the field showing the effectiveness of the above research approach in the synthesis of quantum materials and to foster an open discussion on new research perspectives. We propose that the workshop comprises two 30' invited talks, four 15' contributed talks and a poster session.

**Références**

1. Marzari, N., Ferretti, A. & Wolverton, C. *Electronic-structure methods for materials design*. Nat. Mater. **20**, 736–749 (2021). <https://doi.org/10.1038/s41563-021-01013-3>
2. Vergniory, M.G., Elcoro, L., Felser, C. *et al.* *A complete catalogue of high-quality topological materials*. Nature **566**, 480–485 (2019). <https://doi.org/10.1038/s41586-019-0954-4>
3. A. Marrazzo, M. Gibertini, D. Campi, N. Mounet, and N. Marzari, *Prediction of a Large-Gap and Switchable Kane-Mele Quantum Spin Hall Insulator*, Phys. Rev. Lett. **120**, 117701 (2018).
4. Wang, Wudi; Kim, Stephan; Liu, Minhao; Cevallos, F. A.; Cava, R. J.; Ong, N. P., *Evidence for an edge supercurrent in the Weyl superconductor MoTe<sub>2</sub>*, Science **368**, 534-537 (2020). DOI: [10.1126/science.aaw9270](https://doi.org/10.1126/science.aaw9270)
5. Jian Yu, Mitsuru Itoh, *Physics-Guided Data-Mining Driven Design of Room-Temperature Multiferroic Perovskite Oxides*, Physica Status Solidi **13**, 1900028 (2019). <https://doi.org/10.1002/pssr.201900028>