Computational Quantum Materials

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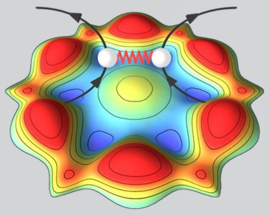

Research topics

- Theory of interacting electron systems
- Topological states of matter
- Realistic calculations of quantum materials
- Computational methods for strongly correlated fermions

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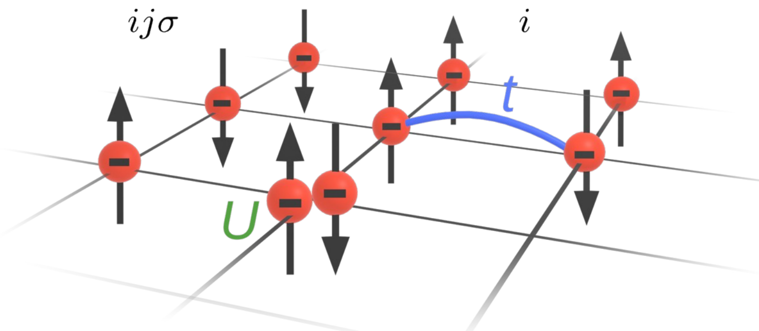
Theory of strongly correlated electrons

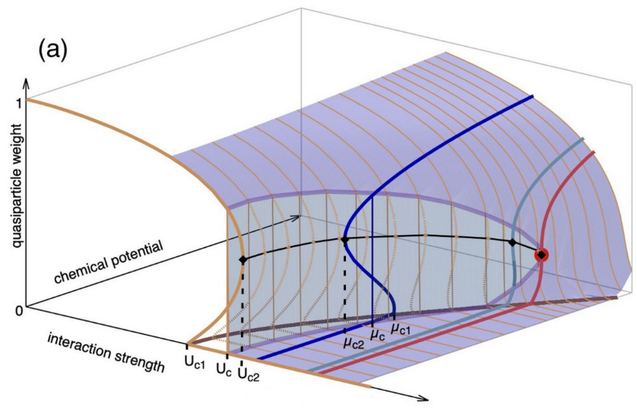
We study strongly correlated electrons, which are described by the simple-looking but hard to solve **Hubbard model**:

$$H = \sum_{ij\sigma} t_{ij} c^\dagger_{i\sigma} c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}$$



including also spin-orbit interaction and multi-orbital effects

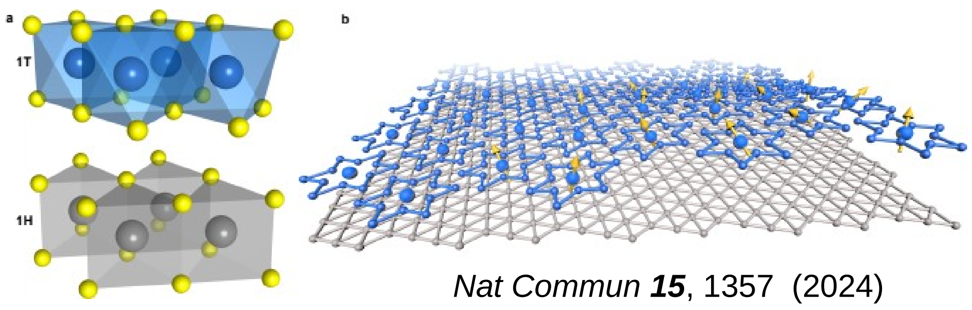
Adding interactions between different orbitals leads to **Hund's physics** which we study using **dynamical mean-field theory (DMFT) + cluster and diagrammatic extensions thereof.**



PRL **130**, 066401 (2023), arXiv:2309.11108 (2023)

Many-body effects in van-der-Waals heterostructures

Stacking and twisting **two-dimensional materials** can lead to interesting correlation effects.

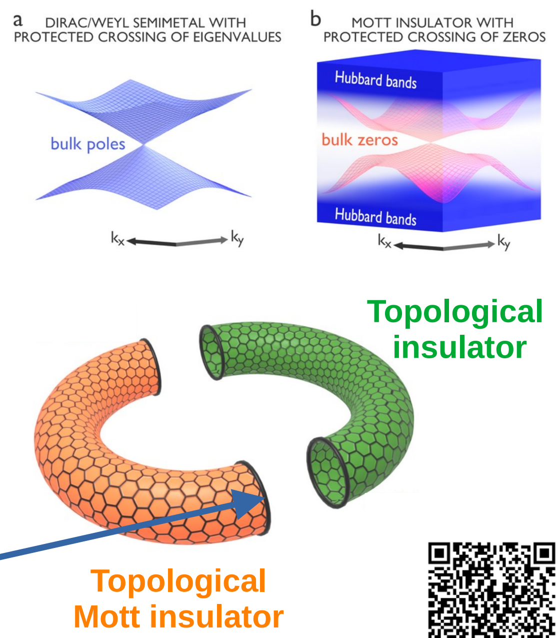


Nat Commun **15**, 1357 (2024)

Example of transition metal dichalcogenides. For magic-angle twisted-bilayer graphene see *PRL* **131**, 166501 (2023) and arXiv:2309.08529

Very strong interactions can open a gap in the electron spectrum (Mott insulator). Inside the gap the **zeros of the Green's function (red)** display surprising topological properties.

The **boundary** of topological Mott insulators hosts **exotic states.**



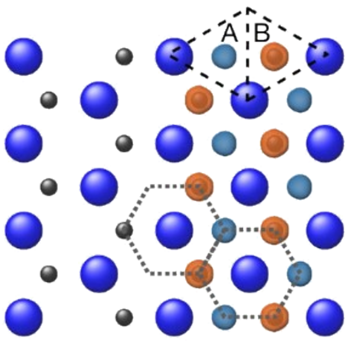
Nat Commun **14,** 7531 (2023), arXiv:2312.13226 (2023)

Quantum Materials

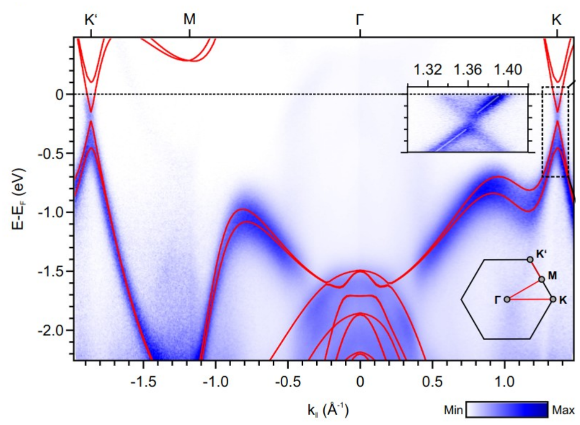
We use **Density Functional Theory (DFT)** to compute realistic band structures of quantum materials.

Indenene

the first of a new family of quantum spin-Hall insulators



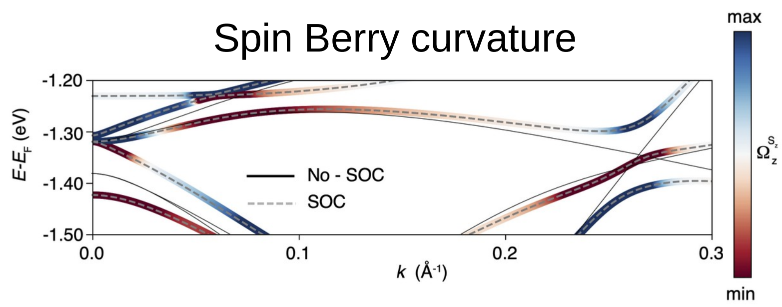
Nat Commun **12**, 5396 (2021)



DFT calculations in perfect agreement with photoemission spectra from EP4 for Indenene

Kagome metals

Spin Berry curvature



PRL **127**, 177001 (2021)
Nat. Phys. **18**, 301–308 (2022)
Nat. Phys. **19**, 1135–1142 (2023)
arXiv:2312.04445 (*Nat. Phys.* in press)