Quantum materials design: challenges and opportunities

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Unconventional superconductivity with high critical temperatures, topologically non-trivial phases, frustrated magnetism, spin-liquids or the recently discussed Kitaev phases are a few examples of exotic states in quantum materials. One of the big challenges in quantum physics is the microscopic description of such materials. Moreover, being able to understand them implies the possibility of predicting compounds with desirable properties. In this talk, I will present and discuss strategies for designing quantum materials from first principles, with emphasis on two-dimensional topological systems (Fig. 1, Fig. 2) [1,2,3] and will motivate their possible use for present technological applications such as quantum computing purposes.

REFERENCES

[1] S. Biswas *et al.* Phys. Rev. Lett. 123 (2019) 237201.
[2] V. Leeb *et al*. Phys. Rev. Lett. 126 (2021) 097201.
[3] J. M. Pizarro *et al.* njp Quantum Materials 5 (2020) 79.

FIGURES

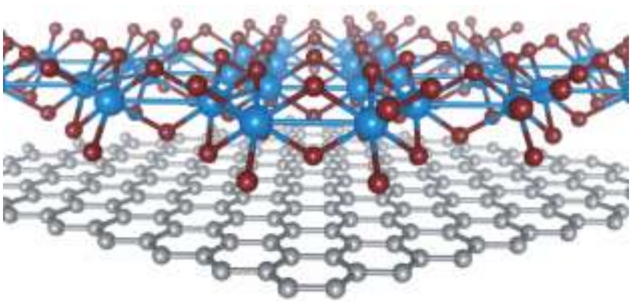

Figure 1: α-$RuCl_3$ in proximity to graphene

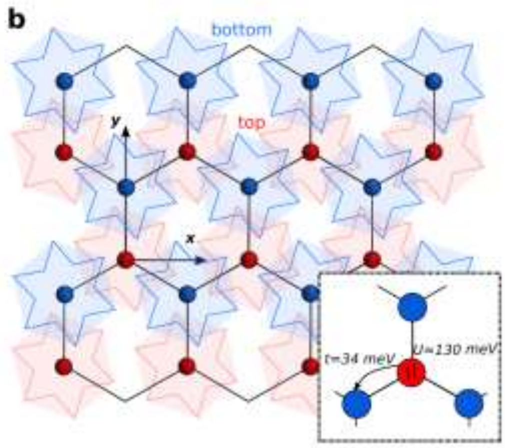

Figure 2: Stacking1T-$TaSe_2$ into bilayers can deconfine electrons from a deep Mott insulating state in the monolayer to a system of correlated Dirac fermions in the bilayer.