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## ABSTRACT:

### A Tale of Cuprates: The Good, the Bad and the Ugly

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The quest for room-temperature multiferroics, materials that simultaneously exhibit magnetic and electric orders, remains one of the grand challenges in condensed matter physics and materials science. In this talk, I will recount my personal journey through the fascinating and sometimes treacherous landscape of copper-based oxides and halides, guided by first-principles calculations and inspired by the spirit of a Spaghetti Western.

Focusing on three cuprate protagonists, CuO [1-3], BaCuF<sub>4</sub> [4], and Cu<sub>2</sub>OCl<sub>2</sub> [5], I will illustrate the full spectrum of outcomes encountered in the computational search for novel multiferroics, from promising discoveries to instructive dead ends. Taken together, these three materials paint a vivid picture of the delicate interplay between spin, lattice, and orbital degrees of freedom that governs the emergence of multiferroicity, shedding light on what it truly takes to find the next room-temperature multiferroic.

[1] Rocquefelte X., Schwarz K., Blaha P. Theoretical investigation of the magnetic exchange interactions in copper(II) oxides under chemical and physical pressures. *Sci. Rep.* 2012;2:759. <https://doi.org/10.1038/srep00759>

[2] Rocquefelte X., Schwarz K., Blaha P., Kumar S., van den Brink J. Room-temperature spin-spiral multiferroicity in high-pressure cupric oxide. *Nat. Commun.* 2013;4:2511. <https://doi.org/10.1038/ncomms3511>

[3] Lafargue-Dit-Hauret W., Braithwaite D., Huxley A.D., Kimura T., Saúl A., Rocquefelte X. Potential room-temperature multiferroicity in cupric oxide under high pressure. *Phys. Rev. B* 2021;103(21):214432. <https://doi.org/10.1103/PhysRevB.103.214432>

[4] Vincent D., Rocquefelte X., Saúl A. Ab initio investigation of the magnetic and ferroelectric properties of BaCuF<sub>4</sub> under hydrostatic pressure. *Phys. Rev. B* 2022;106(6):064421. <https://doi.org/10.1103/PhysRevB.106.064421>

[5] Lafargue-Dit-Hauret W., Rocquefelte X. Influence of the chemical pressure on the magnetic properties of the mixed anion cuprates Cu<sub>2</sub>OX<sub>2</sub> (X = Cl, Br, I). *Computation* 2022;10(5):73. <https://doi.org/10.3390/computation10050073>