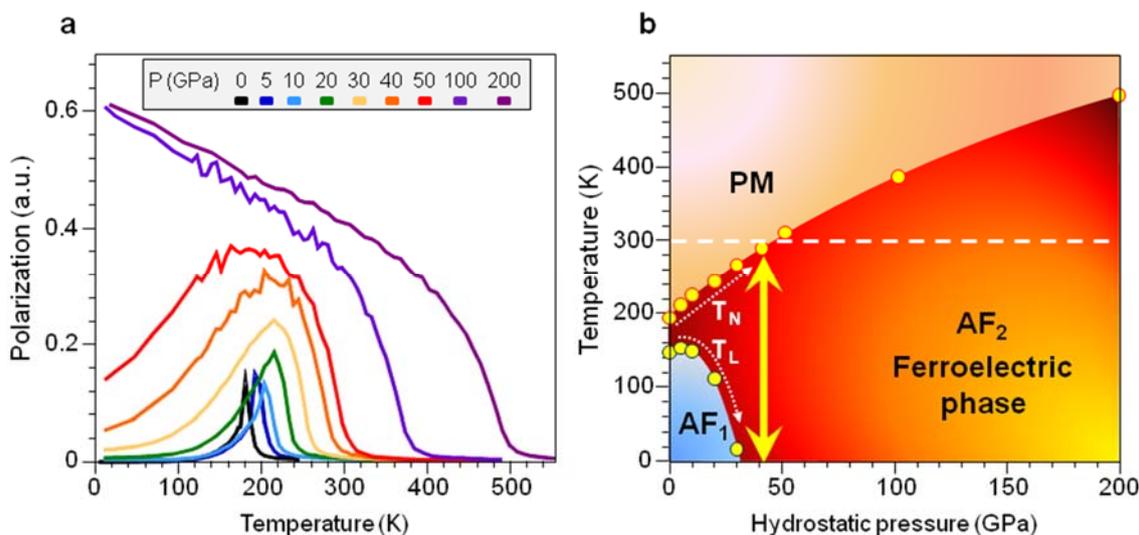


Magnetism and multiferroism in cupric oxide under very high pressure

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Multiferroic materials [1], in which ferroelectric and magnetic ordering coexist, are of fundamental interest for the development of multi-state memory devices that allow for electrical writing and non-destructive magnetic readout operation. The great challenge is to create multiferroic materials that operate at room temperature and have a large ferroelectric polarization P . Cupric oxide, CuO, is promising because it exhibits a significant polarization, that is, $P \sim 0.1 \mu\text{C cm}^{-2}$, for a spin-spiral multiferroic [2]. Unfortunately, CuO is only ferroelectric in a temperature range of 20 K, from 210 to 230 K. Here we propose an original theoretical investigation of the magnetic and ferroelectric properties of CuO under high-pressure based on first-principles and Monte-Carlo calculations. We have established that pressure-driven phase competition renders CuO multiferroic at room-temperature [3-7], while preserving its large polarization and strong magneto-electric coupling. Moreover, under pressure values of 20-40 GPa the multiferroic phase becomes stable in a very broad temperature domain extending above 300K (from 0 to $T > 300\text{K}$).



- [1] Cheong, S. W. & Mostovoy, M. Multiferroics: a magnetic twist for ferroelectricity, *Nature Mater.* **6**, 13-20 (2007).
- [2] Kimura, T., Sekio, Y., Nakamura, H., Siegrist, T., Ramirez, A. P. Cupric oxide as an induced-multiferroic with high- T_C , *Nature Mater.* **7**, 291-294 (2008).
- [3] Giovannetti, G. *et al.* High- T_C Ferroelectricity Emerging from Magnetic Degeneracy in Cupric Oxide, *Phys. Rev. Lett.* **106**, 026401 (2011).
- [4] Rocquefelte, X., Schwarz, K. & Blaha, P. Comment on "High- T_C Ferroelectricity Emerging from Magnetic Degeneracy in Cupric Oxide", *Phys. Rev. Lett.* **107**, 239701 (2011).
- [5] Rocquefelte, X. *et al.* Short-range magnetic order and temperature-dependent properties of cupric oxide, *J. Phys. Condens. Matter* **21**, 045502 (2010).
- [6] Rocquefelte, X., Schwarz, K. & Blaha, P. Theoretical Investigation of the Magnetic Exchange Interactions in Copper(II) Oxides under Chemical and Physical Pressures, *Scientific Reports* **2**, 759 (2012).
- [7] Rocquefelte, X. *et al.* Room-temperature spin-spiral multiferroicity in high-pressure cupric oxide, *Nature Communications* **4**, 2511 (2013).