Modélisation des propriétés magnétiques et multiferroïques de l'oxyde de cuivre

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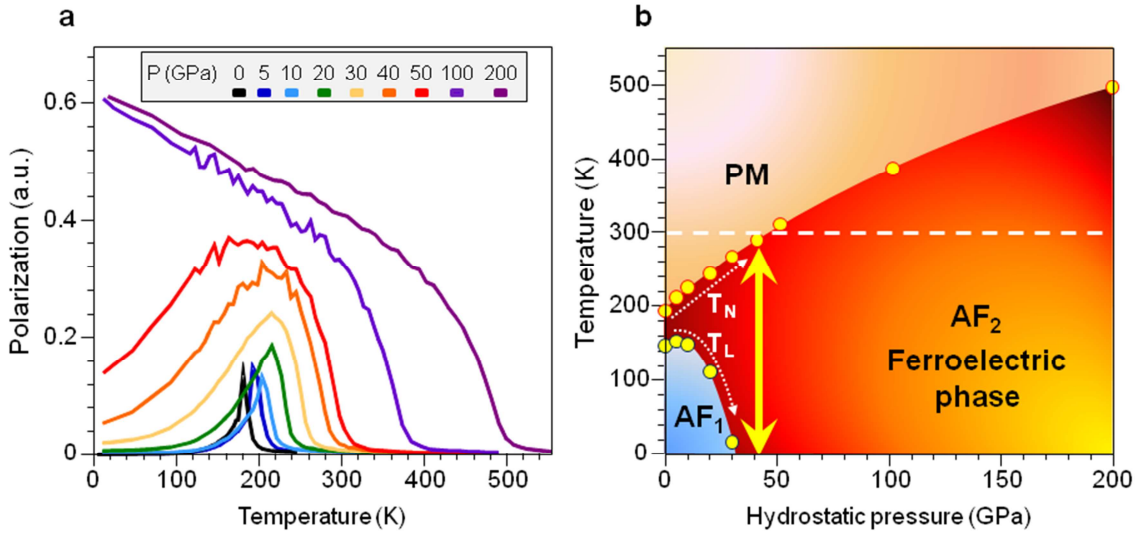
Multiferroic materials [1], in which ferroelectric and magnetic ordering coexist, are of fundamental interest for the development of multi-state memory devices that allow for electrical writing and non-destructive magnetic readout operation. The great challenge is to create multiferroic materials that 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~0.1 µC 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 > 300K).



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