A novel class of molecular and solid state materials with correlated magnetic and dielectric bistability

Pablo Garcia-Fernandez and Isaac B. Bersuker

1Departamento de Ciencias de la Tierra y Física de la Materia Condensada Universidad de Cantabria, Avda. de los Castros s/n. 39005 Santander, Spain

2Institute for Theoretical Chemistry, The University of Texas at Austin, Chemistry and Biochemistry Department, Austin, Texas 78712-0164, USA

Abstract

Materials with switchable properties are most important for information storage, sensors, molecular motors, and spintronic devices. Existing materials usually have the required two stable configurations (bistability), but the lifetime of one of them is often too short for applications. We present here a novel (practically inexhaustible) class of molecular (organic and inorganic) and solid state materials with correlated magnetic and dielectric bistabilities and longer lifetimes. The class properties emerge from a common electronic configuration with a half-filled degenerate valence shell in which the pseudo Jahn-Teller effect produces two coexisting stable and switchable configurations, one with high spin and high (non-polar) symmetry and the other with low (zero) spin and low (dipolar, quadrupolar) symmetry. These correlated magnetic-dielectric bistabilities with reasonable lifetimes are confirmed by state-of-the-art ab initio calculations for a variety of molecular systems and solids; they also demonstrate the presence of a giant magnetoelastic effect in LiCuO$_2$ and NaCuO$_2$ crystals.