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| Title:                  | High-Tc ferroelectricity emerging from magnetic degeneracy in cupric oxide   |
| Authors:                | Kumar, Sanjeev (/jspui/browse?type=author&value=Kumar%2C+Sanjeev)  |
| Keywords:               | Ab initio<br>Cupric oxide<br>Density-functional calculations   |
| Issue Date:             | 2011   |
| Publisher:              | American Physical Society  |
| Citation:               | Physical Review Letters, 106 (2), art. no. 026401  |
| Abstract:               | Cupric oxide is multiferroic at unusually high temperatures. From density functional calculations we find that the low-T magnetic phase is paraelectric, and the higher-T one is ferroelectric with a size and direction of polarization in good agreement with experiments. By mapping the ab initio results on to an effective spin model, we show that the system has a manifold of almost degenerate ground states. In the high-T magnetic state noncollinearity and inversion symmetry breaking stabilize each other via the Dzyaloshinskii-Moriya interaction. This leads to an unconventional mechanism for multiferroicity, with the particular property that nonmagnetic impurities enhance the effect. |
| Description:            | Only IISERM authors are available in the record.   |
| URI:                    | <a href="http://prl.aps.org/abstract/PRL/v106/i2/e026401">http://prl.aps.org/abstract/PRL/v106/i2/e026401</a> ( <a href="http://prl.aps.org/abstract/PRL/v106/i2/e026401">http://prl.aps.org/abstract/PRL/v106/i2/e026401</a> )  |
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