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Title:	Microscopic origin of large negative magnetoelectric coupling in $\text{Sr}_{1/2}\text{Ba}_{1/2}\text{MnO}_3$
Authors:	Kumar, Sanjeev (/jspui/browse?type=author&value=Kumar%2C+Sanjeev)
Keywords:	Ab initio Density functionals Ferroelectric polarization
Issue Date:	2012
Publisher:	The American Physical Society
Citation:	Physical Review Letters, 109 (10), art. no. 107601,
Abstract:	With a combined ab initio density functional and model Hamiltonian approach we establish that in the recently discovered multiferroic phase of the manganite $\text{Sr}_{1/2}\text{Ba}_{1/2}\text{MnO}_3$ the polar distortion of Mn and O ions is stabilized via enhanced in-plane Mn-O hybridizations. The magnetic superexchange interaction is very sensitive to the polar bond-bending distortion, and we find that this dependence directly causes a strong magnetoelectric coupling. This novel mechanism for multiferroicity is consistent with the experimentally observed reduced ferroelectric polarization upon the onset of magnetic ordering.
Description:	Only IISERM authors are available in the record.
URI:	<a href="http://prl.aps.org/abstract/PRL/v109/i10/e107601">http://prl.aps.org/abstract/PRL/v109/i10/e107601</a> ( <a href="http://prl.aps.org/abstract/PRL/v109/i10/e107601">http://prl.aps.org/abstract/PRL/v109/i10/e107601</a> )
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