

NICOLA A. SPALDIN

Publications and Presentations

ResearcherID: A-1017-2010; Orcid ID: 0000-0003-0709-9499

BOOKS

Magnetic materials; fundamentals and device applications, Cambridge University Press (2003). ISBN 0 521 81631 9 (hardback), 0 521 01658 4 (paperback).

Magnetic Materials (2nd Edition) Cambridge University Press (2010). ISBN-13:9780511796166 (Adobe eBook Reader), ISBN-13:9780521886697 (hardback).

JOURNAL PUBLICATIONS ($\sim 51,000$ citations; $h = 90$)

- 224.** *Leggett Modes Accompanying Crystallographic Phase Transitions*, Q. N. Meier, D. Hickox-Young, G. Laurita, N. A. Spaldin, J. M. Rondinelli and M. R. Norman, Phys. Rev. X **12**, 011024 (2022).
- 223.** *Liberating a hidden antiferroelectric phase with interfacial electrostatic engineering*, J. A. Mundy, B. F. Grosso, C. A. Heikes, D. Ferenc Segedin, Z. Wang, Y.-T. Shao, C. Dai, B. H. Goodge, Q. N. Meier, C. T. Nelson, B. Prasad, F. Xue, S. Ganschow, D. A. Muller, L. F. Kourkoutis, L.-Q. Chen, W. D. Ratcliff, N. A. Spaldin, R. Ramesh and D. G. Schlom, Sci. Adv. **8**, eabg5860 (2022).
- 222.** *Anti-symmetric Compton scattering in LiNiPO_4 : Towards a direct probe of the magneto-electric multipole moment*, S. Bhowal, D. O'Neill, M. Fechner, N. A. Spaldin, U. Staub, J. Duffy and S. P. Collins, Open Science Europe **1**, 132 (2021).
- 221.** *Untangling the structural, magnetic dipole, and charge multipolar orders in $\text{Ba}_2\text{MgReO}_6$* , A. Mansouri Tehrani and N. A. Spaldin, Phys. Rev. Mater. **5**, 104410 (2021).
- 220.** *Revealing hidden magnetoelectric multipoles using Compton scattering*, S. Bhowal and N. A. Spaldin, Phys. Rev. Research **3** 033185 (2021).
- 219.** *Interplay between ferroelectricity and metallicity in BaTiO_3* , V. F. Michel, T. Eswein and N. A. Spaldin, J. Mat. Chem. C **9**, 8640 (2021).
- 218.** *Crystal responses to general dark matter-electron interactions*, R. Catena, T. Emken, M. Matas, N. A. Spaldin and E. Urdshals, Phys. Rev. Research **3** 033149 (2021).

-
- 217.** *Magnetoelectric coupling of domains, domain walls and vortices in a multiferroic with independent magnetic and electric order*, M. Giraldo, Q. N. Meier, A. Bortis, D. Nowak, N. A. Spaldin, M. Fiebig, M. C. Weber and T. Lottermoser, *Nature Commun.* **12**, 3093 (2021).
- 216.** *Prediction of low-energy phases of BiFeO_3 with large unit cells and complex tilts beyond Glazer notation*, B. F. Grosso and N. A. Spaldin, *Phys. Rev. Mater.* **5**, 054403 (2021).
- 215.** *Layer and spontaneous polarizations in perovskite oxides and their interplay in multiferroic bismuth ferrite*, N. A. Spaldin, I. Efe, M. D. Rossell and C. Gattinoni, *J. Chem. Phys.* **154**, 154702 (2021).
- 214.** *Oxygen vacancies in strontium titanate: A DFT+DMFT study*, J. Souto-Casares, N. A. Spaldin and C. Ederer, *Phys. Rev. Research* **3**, 023027 (2021).
- 213.** *On the happiness of ferroelectric surfaces and its role in water dissociation: The example of bismuth ferrite*, I. Efe, N. A. Spaldin and C. Gattinoni, *J. Chem. Phys.* **154**, 024702 (2021).
- 212.** *Analogy between the magnetic dipole moment at the surface of a magnetoelectric and the electric charge at the surface of a ferroelectric*, N. A. Spaldin, *JETP* **132**, 493 (2021).
- 211.** *Comparison of coherent phonon generation by electronic and ionic Raman scattering in LaAlO_3* , M. J. Neugebauer, D. M. Juraschek, M. Savoini, P. Engeler, L. Boie, E. Abreu, N. A. Spaldin and S. L. Johnson, *Phys. Rev. Research* **3**, 013126 (2021).
- 210.** *Local Electronic Structure and Dynamics of Muon-Polaron Complexes in Fe_2O_3* , M. H. Dehn, J. K. Shenton, D. J. Arsenau, W. A. MacFarlane, G. D. Morris, A. Maigné, N. A. Spaldin and R. F. Kiefl, *Phys. Rev. Lett.* **126**, 037202 (2021).
- 209.** *In-situ monitoring of interface proximity effects in ultrathin ferroelectrics*, N. Strkalj, C. Gattinoni, A. Vogel, M. Campanini, R. Haerdi, A. Rossi, M. D. Rossell, N. A. Spaldin, M. Fiebig and M. Trassin, *Nature Commun.* **11**, 5815 (2020).
- 208.** *Interface and surface stabilization of the polarization in ferroelectric thin films*, C. Gattinoni, N. Strkalj, R. Härdi, M. Fiebig, M. Trassin, and N. A. Spaldin, *Proc. Natl. Acad. Sci.* 202007736 (2020).
- 207.** *Making EuO multiferroic by epitaxial strain engineering*, V. Goian, R. Held, E. Bousquet, Y. Yuan, A. Melville, H. Zhou, V. Gopalan, Ph. Ghosez, N. A. Spaldin, D. G. Schlom and S. Kamba, *Commun. Mater.* **1:74** (2020).
- 206.** *Phono-magnetic analogs to opto-magnetic effects*, D. M. Juraschek, P. Narang and N. A. Spaldin, *Phys. Rev. Research* **2**, 043035 (2020).

-
- 205.** *Longitudinal and transverse electron paramagnetic resonance in a scanning tunneling microscope*, T. S. Seifert, S. Kovarik, D. M. Juraschek, N. A. Spaldin, P. Gambardella and S. Stepanow, *Science Advances* **6**, eabc5511 (2020).
- 204.** *Theoretical investigation of twin boundaries in WO_3 : Structure, properties, and implications for superconductivity*, N. Mascello, N. A. Spaldin, A. Narayan and Q. N. Meier, *Phys. Rev. Research* **2**, 033460 (2020).
- 203.** *Atomic responses to general dark matter-electron interactions*, R. Catena, T. Emken, N. A. Spaldin and W. Tarantino, *Phys. Rev. Research* **2**, 033195 (2020).
- 202.** *Manifestation of structural Higgs and Goldstone modes in the hexagonal manganites*, Q. N. Meier, A. Stucky, J. Teyssier, S. M. Griffin, D. van der Marel, and N. A. Spaldin, *Phys. Rev. B* **102**, 014102 (2020).
- 201.** *Concepts from the linear magnetoelectric effect that might be useful for antiferromagnetic spintronics*, F. Thöle, A. Keliri and N. A. Spaldin, *J. Appl. Phys.* **127**, 213905 (2020).
- 200.** *Hidden, entangled and resonating order*, G. Aeppli, A. V. Balatsky, H. M. Rønnow and N. A. Spaldin, *Nat. Rev. Mater.* **5**, 477 (2020).
- 199.** *Unconventional Spin Relaxation Involving Localized Vibrational Modes in Ho Single-Atom Magnets*, F. Donati, S. Rusponi, S. Stepanow, L. Persichetti, A. Singha, D. M. Juraschek, C. Wäckerlin, R. Baltic, M. Pivetta, K. Diller, C. Nistor, J. Dreiser, K. Kummer, E. Velez-Fort, N. A. Spaldin, H. Brune, and P. Gambardella, *Phys. Rev. Lett.* **124**, 077204 (2020).
- 198.** *Observation of a Charge-Neutral Muon-Polaron Complex in Antiferromagnetic Cr_2O_3* , M. H. Dehn, J. K. Shenton, S. Holenstein, Q. N. Meier, D. J. Arseneau, D. L. Cortie, B. Hitti, A. C. Y. Fang, W. A. MacFarlane, R. M. L. McFadden, G. D. Morris, Z. Salman, H. Luetkens, N. A. Spaldin, M. Fechner, and R. F. Kiefl, *Phys. Rev. X* **10**, 011036 (2020).
- 197.** *Multiferroics beyond electric-field control of magnetism*, N. A. Spaldin, *Proc. Roy. Soc. A* **476**, 0542 (2020).
- 196.** *The ultrathin limit of improper ferroelectricity*, J. Nordlander, M. Campanini, M. D. Rossell, R. Erni, Q. N. Meier, A. Cano, N. A. Spaldin, M. Fiebig and M. Trassin, *Nature Commun.* **10**, 1 (2019).
- 195.** *Depolarizing-Field Effects in Epitaxial Capacitor Heterostructures*, N. Strkalj, G. De Luca, M. Campanini, S. Pal, J. Schaab, C. Gattinoni, N. A. Spaldin, M. D. Rossell, M. Fiebig and M. Trassin, *Phys. Rev. Lett.* **123**, 147601 (2019).
- 194.** *Dynamical magnetic field accompanying the motion of ferroelectric domain walls*, D. M. Juraschek, Q. N. Meier, M. Trassin, S. E. Trolier-McKinstry, C. L. Degen, and N. A. Spaldin, *Phys. Rev. Lett.* **123**, 127601 (2019).

-
193. *DFT+DMFT study of oxygen vacancies in a Mott insulator*, J. Souto-Casares, N. A. Spaldin and C. Ederer, Phys. Rev. B **100**, 085146 (2019).
192. *Origin and evolution of ferroelectricity in the layered rare-earth-titanate, $R_2Ti_2O_7$, Carpy-Galy phases*, M. Nuñez Valdez and N. A. Spaldin, Polyhedron **171**, 181 (2019).
191. *Ultrafast transient increase of oxygen octahedral rotations in a perovskite*, M. Porer, M. Fechner, M. Kubli, M. J. Neugebauer, S. Parchenko, V. Esposito, A. Narayan, N. A. Spaldin, R. Huber, M. Radovic, E. M. Bothschafter, J. M. Glowia, T. Sato, S. Song, S. L. Johnson and U. Staub, Phys. Rev. Research **1**, 012005R (2019).
190. *Unconventional continuous structural disorder at the order-disorder phase transition in the hexagonal manganites*, S. H. Skjaervo, Q. N. Meier, M. Feygenson, N. A. Spaldin, S. J. L. Billinge, E. S. Bozin and S. M. Selbach, Phys. Rev. X **9**, 031001 (2019).
189. *Orbital magnetic moments of phonons*, D. M. Juraschek and N. A. Spaldin, Phys. Rev. Mater. **3**, 064405 (2019).
188. *Advances in magnetoelectric multiferroics*, N. A. Spaldin and R. Ramesh, Nature Materials **18**, 203 (2019).
187. *Multiferroic quantum criticality*, A. Narayan, A. Cano, A. V. Balatsky and N. A. Spaldin, Nature Materials **18**, 223 (2019).
186. *Dynamic multiferroicity of a ferroelectric quantum critical point*, K. Dunnett, J.-X. Zhu, N. A. Spaldin, V. Juricic and A. V. Balatsky, Phys. Rev. Lett. **122**, 057208 (2019).
185. *Search for the magnetic monopole at a magnetoelectric surface*, Q. N. Meier, M. Fechner, T. Nozaki, M. Sahashi, Z. Salman, T. Prokscha, A. Suter, P. Schoenherr, M. Lilienblum, P. Borisov, I. E. Dzyaloshinskii, M. Fiebig, H. Luetkens, and N. A. Spaldin, Phys. Rev. X **9**, 011011 (2019).
184. *Emergent room temperature polar phase in $CaTiO_3$ nanoparticles and single crystals*, M. O. Ramirez, T. T. A. Lummen, I. Carrasco, E. Barnes, U. Aschauer, D. Stefanska, A. S. Gupta, C. de las Heras, H. Akamatsu, M. Holt, P. Molina, A. Barnes, R. C. Haislmaier, P. J. Deren, C. Prieto, L. E. Bausa, N. A. Spaldin and V. Gopalan, APL Materials **7**, 011103 (2019).
183. *Strain-induced heteronuclear charge disproportionation in $EuMnO_3$* , U. Aschauer, N. Vonrüti and N. A. Spaldin, Phys. Rev. Mater. **3**, 013601 (2019).
182. *Four-spin ring interaction as a source of unconventional magnetic orders in orthorhombic perovskite manganites*, N. S. Fedorova, A. Bortis, C. Findler, N. A. Spaldin, Phys. Rev. B **98**, 235113 (2018).

-
181. *Magnetoelectric multipoles in metals*, F. Thöle and N. A. Spaldin, *Phil. Trans. Roy. Soc. A* **376**, 2017040 (2018).
180. *Oxygen vacancies in the bulk and at neutral domain walls in hexagonal YMnO₃*, S. H. Skjaervo, D. R. Smabraton, N. A. Spaldin, T. Tybell and S. M. Selbach, *Phys. Rev. B* **98**, 184102 (2018).
179. *Evidence of incoherent carriers associated with resonant impurity levels and their influence on superconductivity in the anomalous superconductor Pb_{1-x}Tl_xTe*, P. Giraldo-Gallo, P. Walmsley, B. Sangiorgio, S. C. Riggs, R. D. McDonald, L. Buchauer, B. Fauqué, C. Liu, N. A. Spaldin, A. Kaminski, K. Behnia and I. R. Fisher, *Phys. Rev. Lett.* **121**, 207001 (2018).
178. *Relationship between crystal structure and multiferroic orders in orthorhombic perovskite manganites*, N. S. Fedorova, Y. W. Windsor, C. Findler, M. Ramakrishnan, A. Bortis, L. Rettig, K. Shimamoto, E. M. Bothschafter, M. Porer, V. Esposito, Y. Hu, A. Alberca, T. Lippert, C. W. Schneider, U. Staub and N. A. Spaldin, *Phys. Rev. Mater.* **2**, 104414 (2018).
177. *Emphanitic anharmonicity in PbSe at high temperature and anomalous electronic properties in the Pb Q (Q = S, Se, Te) system*, R. Yu, E. S. Bozin, M. Abeykoon, B. Sangiorgio, N. A. Spaldin, C. D. Malliakas, M. G. Kanatzidis, and S. J. L. Billinge, *Phys. Rev. B* **98**, 144108 (2018).
176. *Correlated local dipoles in PbTe*, B. Sangiorgio, E. S. Bozin, C. D. Malliakas, M. Fechner, A. Simonov, M. G. Kanatzidis, S. J. L. Billinge, N. A. Spaldin, and T. Weber, *Phys. Rev. Mater.* **2**, 085402 (2018).
175. *Magnetophononics: Ultrafast spin control through the lattice*, M. Fechner, A. Sukhov, L. Chotorlishvili, C. Kenel, J. Berakdar and N. A. Spaldin, *Phys. Rev. Mater.* **2**, 064401 (2018).
174. *Strain and ferroelectric soft-mode induced superconductivity in strontium titanate*, K. Dunnnett, A. Narayan, N. A. Spaldin and A. V. Balatsky, *Phys. Rev. B* **97**, 144506 (2018).
173. *Multiferroic magnetic spirals induced by random magnetic exchanges*, A. Scaramucci, H. Shinaoka, M. V. Mostovoy, M. Müller, C. Mudry, M. Troyer and N. A. Spaldin, *Phys. Rev. X* **8**, 011005 (2018).
172. *Fundamental materials research and the course of human civilization*, N. Spaldin, *VSH-Bulletin* **2**, 11 (2017).
171. *Global formation of topological defects in the multiferroic hexagonal manganites*, Q. N. Meier, M. Lilienblum, S. M. Griffin, K. Conder, E. Pomjakushina, Z. Yan, E. Bourret, D. Meier, F. Lichtenberg, E. K. H. Salje, N. A. Spaldin, M. Fiebig and A. Cano, *Phys. Rev. X* **7**, 041014 (2017).

-
170. *Sounding out optical phonons*, D. M. Juraschek and N. A. Spaldin, *Science* **357**, 873 (2017).
169. *On the relationship between topological and geometric defects*, S. M. Griffin and N. A. Spaldin, *J. Phys. Condens. Matter* **29**, 343001 (2017).
168. *Dynamical multiferroicity*, D. M. Juraschek, M. Fechner, A. V. Balatsky and N. A. Spaldin, *Phys. Rev. Mater.* **1**, 014401 (2017).
167. *Multiferroics: Past, present, and future*, N. A. Spaldin, *MRS Bulletin* **42**, 385 (2017).
166. *Multiferroics: from the cosmically large to the subatomically small*, N. A. Spaldin, *Nature Reviews Materials* **2**, 17017 (2017).
165. *Functional electronic inversion layers at ferroelectric domain walls*, J. A. Mundy, J. Schaab, Y. Kumagai, A. Cano, M. Stengel, I. P. Krug, D. M. Gottlob, H. Doglanay, M. E. Holtz, R. Held, Z. Yan, E. Bourret, C. M. Schneider, D. G. Schlom, D. A. Muller, R. Ramesh, N. A. Spaldin and D. Meier, *Nature Materials* **16**, 622 (2017).
164. *A density functional theory study of the influence of exchange-correlation functionals on the properties of FeAs*, S. M. Griffin and N. A. Spaldin, *J. Phys. Condens. Matter* **29**, 215604 (2017).
163. *Defect chemistry as a crystal structure design parameter: Intrinsic point defects and Ga substitution in InMnO_3* , S. M. Griffin, M. Reidulff, S. M. Selbach and N. A. Spaldin, *Chem. Mater.* **29**, 2425 (2017).
162. *Strain-engineered oxygen vacancies in CaMnO_3 thin films*, R. U. Chandrasena, W. Yang, Q. Lei, M. U. Delgado-Jaime, K. D. Wijesekara, M. Golalikhani, B. A. Davidson, E. Arenholz, K. Kobayashi, M. Kobata, F. M. F. de Groot, U. Aschauer, N. A. Spaldin, X. Xi and A. X. Gray, *Nanoletters* **17**, 794 (2017).
161. *Ultrafast structure switching through nonlinear phononics*, D. M. Juraschek, M. Fechner, N. A. Spaldin, *Phys. Rev. Lett.* **118**, 054101 (2017).
160. *Effect of intense optical phonon pumping on the structure and electronic properties of yttrium barium copper oxide*, M. Fechner and N. A. Spaldin, *Phys. Rev. B* **94**, 134397 (2016).
159. *Coupling and competition between ferroelectricity, magnetism, strain, and oxygen vacancies in AMnO_3 perovskites*, A. Marthinsen, C. Farber, U. Aschauer, N. A. Spaldin, S. M. Selbach, *MRS Communications* **6**, 182 (2016).
158. *Fermi surface evolution of Na-doped PbTe studied through density functional theory calculations and Shubnikov–de Haas measurements*, P. Giraldo-Gallo, B. Sangiorgio, P. Walmsley, H. J. Silverstein, M. Fechner, S. C. Riggs, T. H. Geballe, N. A. Spaldin, and I. R. Fisher, *Phys. Rev. B* **94**, 195141 (2016).

-
157. *The 2016 oxide electronic materials and oxide interfaces roadmap*, M. Lorenz, M. S. Ramachandra Rao, T. Venkatesan, E. Fortunato, P. Barquinha, R. Branquinho, D. Salgueiro, R. Martins, E. Carlos, A. Liu, F. K. Shan, M. Grundmann, H. Boschker, J. Mukherjee, M. Priyadarshini, N. DasGupta, D. J. Rogers, F. H. Teherani, E. V. Sandana, P. Bove, K. Rietwyk, A. Zaban, A. Veziridis, A. Weidenkaff, M. Muralidhar, M. Murakami, S. Abel, J. Fompeyrine, J. Zuniga-Perez, R. Ramesh, N. A. Spaldin, S. Ostanin, V. Borisov, I. Mertig, V. Lazenka, G. Srinivasan, W. Prellier, M. Uchida, M. Kawasaki, R. Pentcheva, P. Gegenwart, F. Miletto Granozio, J. Fontcuberta and N. Pryds, *J. Phys. D* **49**, 433001 (2016).
156. *Interplay between strain, defect charge state, and functionality in complex oxides*, U. Aschauer and N. A. Spaldin, *Appl. Phys. Lett.* **109**, 031901 (2016).
155. *Strain-induced structural instability in FeRh*, U. Aschauer, R. Braddell, S. A. Brechbühl, P. M. Derlet, and N. A. Spaldin, *Phys. Rev. B* **94**, 014109 (2016).
154. *Magnetoelastic control of magnetism in an artificial multiferroic*, J. Heidler, M. Fechner, R. V. Chopdekar, C. Piamonteze, J. Dreiser, C. A. Jenkins, E. Arenholz, S. Rusponi, H. Brune, N. A. Spaldin and F. Nolting, *Phys. Rev. B* **94**, 014401 (2016).
153. *First-principles calculation and experimental investigation of lattice dynamics in the rare-earth pyrochlores $R_2Ti_2O_7$ ($R = Tb, Dy, Ho$)*, M. Ruminy, M. Nuñez Valdez, B. Wehinger, A. Bosak, D. T. Adroja, U. Stuhr, K. Iida, K. Kamazawa, E. Pomjakushina, D. Prabakharan, M. K. Haas, L. Bovo, D. Sheptyakov, A. Cervellino, R. J. Cava, M. Kenzelmann, N. A. Spaldin and T. Fennell, *Phys. Rev. B* **93**, 214308 (2016).
152. *First-principles calculation of the bulk magnetoelectric monopole density: Berry phase and Wannier function approaches*, F. Thöle, M. Fechner and N. A. Spaldin, *Phys. Rev. B* **93**, 195167 (2016).
151. *Quasistatic magnetoelectric multipoles as order parameter for pseudogap phase in cuprate superconductors*, M. Fechner, M. J. A. Fierz, F. Thöle, U. Staub and N. A. Spaldin, *Phys. Rev. B* **93**, 174419 (2016).
150. *Origin of ferroelectric polarization in tetragonal tungsten-bronze-type oxides*, G. H. Olsen, U. Aschauer, N. A. Spaldin, S. M. Selbach and T. Grande, *Phys. Rev. B* **93**, 180101(R) (2016).
149. *The valence band electronic structure of rhombohedral-like and tetragonal-like $BiFeO_3$ thin films from hard X-ray photoelectron spectroscopy and first-principles theory*, D. Mazumdera, R. Knut, F. Thöle, M. Gorgoi, S. Faleev, O. N. Mryasov, V. Shelke, C. Ederer, N. A. Spaldin, A. Gupta and O. Karis, *J. Elec. Spectroscopy and Related Phenomena* **208**, 63 (2016).

-
148. *A bespoke single-band Hubbard model material*, S. M. Griffin, P. Staar, T. C. Schulthess, M. Troyer and N. A. Spaldin, Phys. Rev. B **93**, 075115 (2016).
147. *Ab initio study of the ferroelectric strain dependence and 180° domain walls in the barium metal fluorides $BaMgF_4$ and $BaZnF_4$* , M. N. Valdez, H. T. Spanke and N. A. Spaldin, Phys. Rev. B **93**, 064112 (2016).
146. *Strain-induced magnetic anisotropy in epitaxial thin films of the spinel $CoCr_2O_4$* , J. A. Heuver, A. Scaramucci, Y. Blickenstorfer, S. Matzen, N. A. Spaldin, C. Ederer and B. Noheda, Phys. Rev. B **92**, 214429 (2015).
145. *Quantum critical origin of the superconducting dome in $SrTiO_3$* , J. M. Edge, Y. Kadem, U. Aschauer, N. A. Spaldin, and A. V. Balatsky, Phys. Rev. Lett. **115**, 247002 (2015).
144. *Effect of epitaxial strain on cation and anion vacancy formation in MnO* , U. Aschauer, N. Vonrüti and N. A. Spaldin, Phys. Rev. B **92**, 054103 (2015).
143. *Strain induced coupling of electrical polarization and structural defects in $SrMnO_3$ films*, C. Becher, L. Maurel, U. Aschauer, M. Lilienblum, C. Magén, D. Meier, E. Langenberg, M. Trassin, J. Blasco, I. P. Krug, P. A. Algarabel, N. A. Spaldin, J. A. Pardo and M. Fiebig, Nature Nanotechnology **10**, 661 (2015).
142. *Find your most interesting question*, N. A. Spaldin, Science **349**, 110 (2015).
141. *Separating different contributions to the crystal-field parameters using Wannier functions*, A. Scaramucci, J. Ammann, N. A. Spaldin and C. Ederer, J. Phys. Condens. Matt. **27**, 75503 (2015).
140. *Biquadratic and ring exchange interactions in orthorhombic perovskite manganites*, N. S. Fedorova, C. Ederer, N. A. Spaldin and A. Scaramucci, Phys. Rev. B **91**, 165122 (2015).
139. *Incommensurate magnetic structure, Fe/Cu chemical disorder, and magnetic interactions in the high-temperature multiferroic $YBaCuFeO_5$* , M. Morin, A. Scaramucci, M. Bartkowiak, E. Pomjakushina, G. Deng, D. Sheptyakov, L. Keller, J. Rodriguez-Carvajal, N. A. Spaldin, M. Kenzelmann, K. Conder and M. Medarde, Phys. Rev. B **91**, 4408 (2015).
138. *Large resistivity modulation in mixed-phase metallic systems*, Y. Lee, Z. Q. Liu, J. T. Heron, J. D. Clarkson, J. Hong, C. Ko, M. D. Biegalski, U. Aschauer, S. L. Hsu, M. E. Nowakowski, J. Wu, H. M. Christen, S. Salahuddin, J. B. Bokor, N. A. Spaldin, D. G. Schlom and R. Ramesh, Nature Commun. **6**, 5959 (2015).
137. *Duality of topological defects in hexagonal manganites*, F.-T. Huang, X. Wang, S. M. Griffin, Y. Kumagai, O. Gindele, C. Ming-Wen, Y. Horibe, N. A. Spaldin and S.-W. Cheong, Phys. Rev. Lett. **113**, 267602 (2014).

-
136. *Nonlinear lattice dynamics as a basis for enhanced superconductivity in $YBa_2Cu_3O_{6.5}$* , R. Mankowsky, A. Subedi, M. Först, S. O. Mariager, M. Chollet, H. T. Lemke, J. S. Robinson, J. M. Glowia, M. P. Minitti, A. Frano, M. Fechner, N. A. Spaldin, T. Loew, B. Keimer, A. Georges and A. Cavalleri, *Nature* **516**, 71 (2014).
135. *Perovskite-structure $TlMnO_3$: A new manganite with new properties*, W. Wei, Y. Kumagai, N. A. Spaldin, Y. Matsushita, A. Sato, I. A. Presniakov, A. V. Sobolev, Y. S. Glazkova and A. A. Belik, *Inorganic Chemistry* **53**, 9800 (2014).
134. *Magnetic field generated by a charge in a uniaxial magnetoelectric material*, M. Fechner, N. A. Spaldin and I. E. Dzyaloshinskii, *Phys. Rev. B* **89**, 184415 (2014).
133. *Competition and cooperation between antiferrodistortive and ferroelectric instabilities in the model perovskite $SrTiO_3$* , U. Aschauer and N. A. Spaldin, *J. Phys. Condens. Matter* **26**, 122203 (2014).
132. *Geometric ferroelectricity in fluoroperovskites*, A. C. Garcia-Castro, N. A. Spaldin, A. H. Romero and E. Bousquet, *Phys. Rev. B* **89**, 104107 (2014).
131. *Landau theory of topological defects in multiferroic hexagonal manganites*, S. Artyukhin, K. T. Delaney, N. A. Spaldin and M. Mostovoy, *Nature Materials* **13**, 42 (2014).
130. *Strong coupling of Jahn-Teller distortion to oxygen-octahedron rotation and functional properties in epitaxially strained orthorhombic $LaMnO_3$* , J. H. Lee, K. T. Delaney, E. Bousquet, N. A. Spaldin and K. M. Rabe, *Phys. Rev. B* **88**, 174426 (2013).
129. *Quantification of octahedral rotations in strained $LaAlO_3$ films via synchrotron x-ray diffraction*, R. L. Johnson-Wilke, D. Marincel, S. Zhu, M. P. Warusawithana, A. Hatt, J. Sayre, K. T. Delaney, R. Engel-Herbert, C. M. Schlepütz, J.-W. Kim, V. Gopalan, N. A. Spaldin, D. G. Schlom, P. J. Ryan, and S. Trolier-McKinstry, *Phys. Rev. B* **88**, 174101 (2013).
128. *Monopole-based formalism for the diagonal magnetoelectric response*, N. A. Spaldin, M. Fechner, E. Bousquet, A. Balatsky and L. Nordström, *Phys. Rev. B* **88**, 094429 (2013).
127. *Functional ion defects in transition metal oxides*, S. V. Kalinin and N. A. Spaldin, *Science* **341**, 858 (2013).
126. *Strain-controlled oxygen vacancy formation and ordering in $CaMnO_3$* , U. Aschauer, R. Pfenninger, S. M. Selbach, T. Grande and N. A. Spaldin, *Phys. Rev. B* **88**, 054111 (2013).

-
125. *Structural and optoelectronic characterization of RF sputtered ZnSnN₂*, L. Lahourcade, N. C. Coronel, K. T. Delaney, S. K. Shukla, N. A. Spaldin and H. A. Atwater, *Adv. Mater.* **25**, 2562 (2013).
 124. *Structural domain walls in polar hexagonal manganites*, Y. Kumagai and N. A. Spaldin, *Nature Commun.* **4**, 1540 (2013).
 123. *Novel nanorod precipitate formation in neodymium and titanium codoped bismuth ferrite*, I. MacLaren, L. Q. Wang, B. Schaffer, Q. M. Ramasse, A. J. Craven, S. M. Selbach, N. A. Spaldin, S. Miao, K. Kalantari and I. M. Reaney, *Advanced Functional Materials* **23**, 683 (2013).
 122. *Translation domains in multiferroics*, D. Meier, M. Lilienblum, P. Becker, L. Bohaty, N. A. Spaldin, R. Ramesh and M. Fiebig, *Phase Transitions* **86**, 33 (2013).
 121. *Scaling behavior and beyond equilibrium in the hexagonal manganites*, S. M. Griffin, M. Lilienblum, K. T. Delaney, Y. Kumagai, M. Fiebig and N. A. Spaldin, *Phys. Rev. X* **2**, 041022 (2012).
 120. *Linear magnetoelectric effect by orbital magnetism*, A. Scaramucci, E. Bousquet, M. Fechner, M. Mostovoy and N. A. Spaldin, *Phys. Rev. Lett.* **109**, 197203 (2012).
 119. *Noncollinear magnetism and single-ion anisotropy in multiferroic perovskites*, C. Weingart, N. A. Spaldin and E. Bousquet, *Phys. Rev. B* **86**, 094413 (2012).
 118. *A beginner's guide to the modern theory of polarization*, N. A. Spaldin, *J. Sol. Stat. Chem.* **195**, 2 (2012).
 117. *Observation of persistent centrosymmetry in the hexagonal manganite family*, Y. Kumagai, A. A. Belik, M. Lilienblum, N. Leo, M. Fiebig and N. A. Spaldin, *Phys. Rev. B* **85**, 174422 (2012).
 116. *Ab initio investigation of FeAs/GaAs heterostructures for potential spintronic and superconducting applications*, S. M. Griffin and N. A. Spaldin, *Phys. Rev. B* **85**, 155126 (2012).
 115. *Anisotropic conductance at improper ferroelectric domain walls*, D. Meier, J. Seidel, A. Cano, K. Delaney, Y. Kumagai, M. Mostovoy, N. A. Spaldin, R. Ramesh and M. Fiebig, *Nature Materials* **11**, 284-288 (2012).
 114. *First-principles prediction of oxygen octahedral rotations in perovskite-structure EuTiO₃*, K. Z. Rushchanskii, N. A. Spaldin and M. Lezaic, *Phys. Rev. B* **85**, 104109 (2012).
 113. *Induced magnetoelectric response in Pnma perovskites*, E. Bousquet and N. A. Spaldin, *Phys. Rev. Lett.* **107**, 197603 (2011).

-
112. *Structure and properties of functional oxide thin films: Insights From Electronic-Structure Calculations*, J. M. Rondinelli and N. A. Spaldin, *Adv. Mater.* **23**, 3363 (2011).
 111. *High-temperature multiferroicity and strong magnetocrystalline anisotropy in 3d – 5d double perovskites*, M. Lezaic and N. A. Spaldin, *Phys. Rev. B* **83**, 24410 (2011).
 110. *Band alignment at metal/ferroelectric interfaces: Insights and artifacts from first principles*, M. Stengel, P. Aguado-Puente, N. A. Spaldin and J. Junquera, *Phys. Rev. B* **83**, 235112 (2011).
 109. *Shedding light on oxide interfaces*, G. Hammerl and N. A. Spaldin, *Science* **332**, 925-926 (2011).
 108. *Stress-induced R-M-A-M-C-T symmetry changes in BiFeO₃ films*, H. M. Christen, J. H. Nam, H. S. Kim, A. J. Hatt and N. A. Spaldin, *Phys. Rev. B* **83**, 144107 (2011).
 107. *Unexpectedly large electronic contribution to linear magnetoelectricity*, E. Bousquet, N. A. Spaldin and K. T. Delaney, *Phys. Rev. Lett.* **106**, 107202 (2011).
 106. *Entropically stabilized local dipole formation in lead chalcogenides*, E. S. Bozin, C. D. Malliakas, P. Souvatzis, T. Proffen, N. A. Spaldin, M. G. Kanatzidis and S. J. L. Billinge, *Science* **330**, 1660 (2010).
 105. *J-dependence in the LSDA+U treatment of noncollinear magnets* E. Bousquet and N. A. Spaldin, *Phys. Rev. B* **82**, 220402(R) (2010). *Editor's Choice*
 104. *Multiferroics: Past, present, and future*, N. A. Spaldin, S.-W. Cheong and R. Ramesh, *Physics Today* **63**, 38 (2010).
 103. *Structural phases of strained LaAlO₃ driven by octahedral tilt instabilities*, A. J. Hatt and N. A. Spaldin, *Phys. Rev. B* **82**, 195402 (2010).
 102. *Electric and magnetic polarizabilities of hexagonal Ln₂CuTiO₆ (Ln=Y, Dy, Ho, Er, and Yb)*, D. Choudhury, A. Hazarika, A. Venimadhav, C. Kakarla, K. T. Delaney, P. Sujatha Devi, P. Mondal, R. Nirmala, J. Gopalakrishnan, N. A. Spaldin, U. V. Waghmare, and D. D. Sarma, *Phys. Rev. B* **82**, 134203 (2010).
 101. *Temperature-dependent magnetoelectric effect from first principles*, M. Mostovoy, A. Scaramucci, N. A. Spaldin and K. T. Delaney, *Phys. Rev. Lett.* **105**, 087202 (2010).
 100. *Substrate coherency driven octahedral rotations in perovskite oxide films*, J. M. Rondinelli and N. A. Spaldin, *Phys. Rev. B* **82**, 113402 (2010).
 99. *Quantifying octahedral rotations in strained perovskite oxide films*, S. J. May, J.-W. Kim, J. M. Rondinelli, E. Karapetrova, N. A. Spaldin, A. Bhattacharya and P. J. Ryan, *Phys. Rev. B* **82**, 014110 (2010).

-
98. *A multiferroic material to search for the permanent electric dipole moment of the electron*, K. Z. Rushchanskii, S. Kamba, V. Goian, P. Vaněk, M. Savinov, J. Prokleška, D. Nuzhnyy, K. Knížek, F. Laufek, S. Eckel, S. K. Lamoreaux, A. O. Sushkov, M. Ležaić and N. A. Spaldin, *Nature Materials* **9**, 649 (2010).
97. *Chemical control of polar behavior in bicomponent short-period superlattices*, H. Das, N. A. Spaldin, U. V. Waghmare and T. Saha-Dasgupta, *Phys. Rev. B* **81**, 235112 (2010).
96. *Unusual dielectric response in B-site size-disordered hexagonal transition metal oxides*, D. Choudhury, A. Venimadhav, C. Kakarla, K. T. Delaney, P. S. Devi, P. Mondal, R. Nirmala, J. Gopalakrishnan, N. A. Spaldin, U. V. Waghmare, and D. D. Sarma, *Appl. Phys. Lett.* **96**, 162903 (2010).
95. *Theoretical study of Schottky-barrier formation at epitaxial rare-earth-metal/semiconductor interfaces*, K. Delaney, N. A. Spaldin and C. G. van de Walle, *Phys. Rev. B* **81**, 165312 (2010).
94. *Electron-lattice instabilities suppress cuprate-like electronic structures in SrFeO₃/SrTiO₃ superlattices*, J. M. Rondinelli and N. A. Spaldin, *Phys. Rev. B* **81**, 085109 (2010).
93. *Strain-induced isosymmetric phase transition in BiFeO₃*, A. J. Hatt, N. A. Spaldin and C. Ederer, *Phys. Rev. B* **81**, 054109 (2010).
92. *Strain-induced ferroelectricity in simple rocksalt binary oxides*, E. Bousquet, N. A. Spaldin and Ph. Ghosez, *Phys. Rev. Lett.* **104**, 037601 (2010).
91. *Mn³⁺ in trigonal bipyramidal coordination: A new blue chromophore* A. E. Smith, H. Mizoguchi, K. Delaney, N. A. Spaldin, A. W. Sleight and M. A. Subramanian, *J. Am. Chem. Soc.* **131**, 17084 (2009).
90. *First-principles modeling of ferroelectric capacitors via constrained displacement field calculations*, M. Stengel, D. Vanderbilt and N. A. Spaldin, *Phys. Rev. B* **80**, 224110 (2009). *Editor's Choice*
89. *A strain-driven morphotropic phase boundary in BiFeO₃*, R. J. Zeches, M. D. Rossell, J. X. Zhang, A. J. Hatt, Q. He, C.-H. Yang, A. Kumar, C. H. Wang, A. Melville, C. Adamo, G. Sheng, Y.-H. Chu, J. F. Ihlefeld, R. Erni, C. Ederer, V. Gopalan, L. Q. Chen, D. G. Schlom, N. A. Spaldin, L. W. Martin and R. Ramesh, *Science* **326**, 977 (2009).
88. *Current trends of the magnetoelectric effect*, M. Fiebig and N. A. Spaldin, *Eur. Phys. J. B* **71**, 293 (2009).
87. *Strain effects on the electric polarization of BiMnO₃*, A. J. Hatt and N. A. Spaldin, *Eur. Phys. J. B* **71**, 435 (2009).

-
86. *First-principles study of ferroelectric domain walls in multiferroic bismuth ferrite*, A. Lubk, S. Gemming and N. A. Spaldin, Phys. Rev. B **80**, 104110 (2009). *Editor's Choice*
85. *Non- d^0 Mn-driven ferroelectricity in antiferromagnetic $BaMnO_3$* , J. M. Rondinelli, A. S. Eidelson and N. A. Spaldin, Phys. Rev. B **79**, 205119 (2009). *Editor's Choice*
84. *Enhancement of ferroelectricity at metal/oxide interfaces*, M. Stengel, D. Vanderbilt and N. A. Spaldin, Nature Materials, **8**, 392 (2009).
83. *Superexchange-driven magnetoelectricity in magnetic vortices*, K. T. Delaney, M. Mostovoy and N. A. Spaldin, Phys. Rev. Lett. **102**, 157203 (2009).
82. *Role of atomic multiplets in the electronic structure of rare-earth semiconductors and semimetals*, L. V. Pourovskii, K. T. Delaney, C. G. Van de Walle, N. A. Spaldin, and A. Georges, Phys. Rev. Lett. **102**, 096401 (2009).
81. *Electric displacement as the fundamental variable in electronic-structure calculations*, M. Stengel, N. A. Spaldin and D. Vanderbilt, Nature Physics **5**, 304 (2009).
80. *Conduction at domain walls in oxide multiferroics*, J. Seidel, L. W. Martin, Q. He, Q. Zhan, Y.-H. Chu, A. Rother, M. E. Hawkrige, P. Maksymovych, P. Yu, M. Gajek, N. Balke, S. V. Kalinin, S. Gemming, F. Wang, G. Catalan, J. F. Scott, N. A. Spaldin, J. Orenstein and R. Ramesh, Nature Materials **8**, 229 (2009).
79. *Structural effects on the spin-state transition in epitaxially strained $LaCoO_3$ films*, J. M. Rondinelli and N. A. Spaldin, Phys. Rev. B **79**, 054409 (2009).
78. *Electric field control of magnetism in complex oxide thin films*, N. A. Spaldin and R. Ramesh, MRS Bulletin **33**, 1047 (2008).
77. *The toroidal moment in condensed-matter physics and its relation to the magnetoelectric effect*, N. A. Spaldin, M. Fiebig and M. Mostovoy, J. Phys. Condens. Matter **20**, 434203 (2008).
76. *Electronic properties of bulk and thin film $SrRuO_3$: Search for the metal-insulator transition*, J. M. Rondinelli, N. M. Caffrey, S. Sanvito and N. A. Spaldin, Phys. Rev. B **78**, 155107 (2008).
75. *Theoretical study of the structural and electronic properties of strained $ErAs$* , K. T. Delaney, N. A. Spaldin and C. G. Van de Walle, Phys. Rev. B **77**, 235117 (2008).
74. *Self-interaction correction with Wannier functions*, M. Stengel and N. A. Spaldin, Phys. Rev. B **77**, 155106 (2008).
73. *Carrier-mediated magnetoelectricity in complex oxide heterostructures*, J. M. Rondinelli, M. Stengel and N. A. Spaldin, Nature Nanotechnology **3**, 46 (2008).

-
72. *Towards a microscopic theory of toroidal moments in bulk periodic crystals*, C. Ederer and N. A. Spaldin, Phys. Rev. B **76**, 214404 (2007).
71. *Analogies and differences between ferroelectrics and ferromagnets*, N. A. Spaldin, Topics in Applied Physics **105**, 175 (2007).
70. *Ferrodistoritive instability at the (001) surface of half-metallic manganites*, J. M. Pruneda, V. Ferrari, R. Rurali, P. B. Littlewood, N. A. Spaldin and E. Artacho, Phys. Rev. Lett. **99**, 226101 (2007).
69. *Anti-polarity in ideal BiMnO₃*, P. Baettig, R. Seshadri and N. A. Spaldin, J. Am. Chem. Soc. **129**, 9854-9855 (2007).
68. *Density-functional investigation of the (113)[-110] twin grain boundary in Co-doped anatase TiO₂ and its influence on magnetism in dilute magnetic semiconductors*, S. Gemming, R. Janisch, M. Schreiber and N. A. Spaldin, Phys. Rev. B **76**, 045204 (2007).
67. *Tri-layer superlattices: A route to magnetoelectric multiferroics?* A. J. Hatt and N. A. Spaldin, Appl. Phys. Lett. **90**, 242916 (2007).
66. *Ab initio theory of metal-insulator interfaces in a finite electric field*, M. Stengel and N. A. Spaldin, Phys. Rev. B **75**, 205121 (2007).
65. *Multiferroics: Progress and prospects in thin films*, R. Ramesh and N. A. Spaldin, Nature Materials **6**, 21 (2007).
64. *Mott transition of MnO under pressure: A comparison of correlated band theories*, D. Kasinathan, J. Kunes, K. Koepernik, C. V. Diaconu, R. L. Martin, I. D. Prodan, G. E. Scuseria, N. A. Spaldin, L. Petit, T. C. Schulthess and W. E. Pickett, Phys. Rev. B **74**, 195110 (2006).
63. *Origin of the dielectric dead layer in nanoscale capacitors*, M. Stengel and N. A. Spaldin, Nature **443**, 679 (2006).
62. *Electrical control of antiferromagnetic domains in multiferroic BiFeO₃ films at room temperature*, T. Zhao, A. Scholl, F. Zavaliche, K. Lee, M. Barry, A. Doran, M. P. Cruz, Y. H. Chu, C. Ederer, N. A. Spaldin, R. R. Das, D. M. Kim, S. H. Baek, C. B. Eom and R. Ramesh, Nature Materials **5**, 823 (2006).
61. *Magnetic interactions in transition-metal-doped ZnO: An ab initio study*, P. Gopal and N. A. Spaldin, Phys. Rev. B **74**, 094418 (2006).
60. *Origin of ferroelectricity in the multiferroic barium fluorides BaMF₄: A first principles study*, C. Ederer and N. A. Spaldin, Phys. Rev. B **74**, 024102 (2006)
59. *Electric-field-switchable magnets: The case of BaNiF₄*, C. Ederer and N. A. Spaldin, Phys. Rev. B **74**, 020401(R) (2006)

-
58. *Lattice relaxation in oxide heterostructures: LaTiO₃/SrTiO₃ superlattices*, S. Okamoto, A. Millis and N. A. Spaldin, Phys. Rev. Lett. **97**, 056802 (2006).
 57. *Polarization, piezoelectric constants and elastic constants of ZnO, MgO and CdO*, P. Gopal and N. A. Spaldin, J. Elec. Mat. **35**, 538 (2006).
 56. *Accurate polarization within a unified Wannier function formalism*, M. Stengel and N. A. Spaldin, Phys. Rev. B **73**, 075121 (2006).
 55. *Understanding ferromagnetism in Co-doped TiO₂ anatase from first principles*, R. Janisch and N. A. Spaldin, Phys. Rev. B **73**, 035201 (2006).
 54. *Recent progress in first-principles studies of magnetoelectric multiferroics*, C. Ederer and N. A. Spaldin, Curr. Opin. Sol. Stat. and Mater. Sci. **9**, 128 (2005).
 53. *First principles study of the multiferroics BiFeO₃, Bi₂FeCrO₆, and BiCrO₃: Structure, polarization, and magnetic ordering temperature*, P. Baettig, C. Ederer and N. A. Spaldin, Phys. Rev. B **72**, 214105 (2005).
 52. *Effect of epitaxial strain on the spontaneous polarization of thin film ferroelectrics*, C. Ederer and N. A. Spaldin, Phys. Rev. Lett. **95**, 257601 (2005).
 51. *The renaissance of magnetoelectric multiferroics*, N. A. Spaldin and M. Fiebig, Science **309**, 391 (2005).
 50. *Transition metal-doped TiO₂ and ZnO – present status of the field*, R. Janisch, P. Gopal and N. A. Spaldin, J. Phys.: Condens. Matter **17**, R657 (2005).
 49. *Influence of strain and oxygen vacancies on the magnetoelectric properties of multiferroic bismuth ferrite*, C. Ederer and N. A. Spaldin, Phys. Rev. B **71**, 224103 (2005).
 48. *Theoretical prediction of new high-performance, lead-free piezoelectrics*, P. Baettig, C. Schelle, R. LeSar, U. Waghmare and N. A. Spaldin, Chem. Mat. **17**, 1376 (2005).
 47. *Strong correlation and ferromagnetism in (Ga,Mn)As and (Ga,Mn)N*, A. Filippetti, N. A. Spaldin and S. Sanvito, J. Mag. Mag. Mat. **290-291**, 1391 (2005).
 46. *Schrödinger’s mousetrap*, N. A. Spaldin, Nature **434**, 25 (2005).
 45. *Weak ferromagnetism and magnetoelectric coupling in bismuth ferrite*, C. Ederer and N. A. Spaldin, Phys. Rev. B **71**, 060401(R) (2005).
 44. *Ab initio prediction of a multiferroic with large polarization and magnetization*, P. Baettig and N. A. Spaldin, Appl. Phys. Lett. **86**, 012505 (2005).

-
43. *First-principles study of spontaneous polarization in multiferroic BiFeO₃*, J. B. Neaton, C. Ederer, U. V. Waghmare, N. A. Spaldin and K. M. Rabe, Phys. Rev. B **71**, 014113 (2005).
 42. *Self-interaction effects in (Ga,Mn)As and (Ga,Mn)N*, A. Filippetti, N. A. Spaldin and S. Sanvito, Chem. Phys. **309**, 59 (2004).
 41. *A new route to magnetic ferroelectrics*, C. Ederer and N. A. Spaldin, Nature Materials **3**, 849 (2004).
 40. *First-principles study of wurtzite-structure MnO*, P. Gopal, N. A. Spaldin and U. V. Waghmare, Phys. Rev. B **70**, 205104 (2004).
 39. *Density-functional study of charge doping in WO₃*, A. D. Walkinshaw, N. A. Spaldin and E. Artacho, Phys. Rev. B **70**, 165110 (2004).
 38. *Fundamental size limits in ferroelectricity*, N. A. Spaldin, Science **304**, 1606 (2004).
 37. *Multiferroic materials tower up*, N. A. Spaldin, Physics World **17** (4), 20 (2004).
 36. *Search for ferromagnetism in transition-metal-doped piezoelectric ZnO*, N. A. Spaldin, Phys. Rev. B **69**, 125201 (2004).
 35. *The origin of ferroelectricity in magnetoelectric YMnO₃*, B. B. Van Aken, T. T. M. Palstra, A. Filippetti and N. A. Spaldin, Nature Materials **3**, 164 (2004).
 34. *Computational design of multifunctional materials*, N. A. Spaldin and W. E. Pickett, J. Sol. Stat. Chem. **176**, 615 (2003).
 33. *Magnetism in polycrystalline cobalt-substituted zinc oxide*, A. S. Risbud, N. A. Spaldin, Z. Q. Chen, S. Stemmer, and R. Seshadri, Phys. Rev. B **68**, 205202 (2003).
 32. *Strong-correlation effects in Born effective charges*, A. Filippetti and N. A. Spaldin, Phys. Rev. B **68**, 045111 (2003).
 31. *Epitaxial BiFeO₃ multiferroic thin film heterostructures*, J. Wang, J. B. Neaton, H. Zheng, V. Nagarajan, S. B. Ogale, B. Liu, D. Viehland, V. Vaithyanathan, D. G. Schlom, U. V. Waghmare, N. A. Spaldin, K. M. Rabe, M. Wuttig and R. Ramesh, Science **299** (5613), 1719 (2003).
 30. *Self-interaction corrected pseudopotential scheme for magnetic and strongly-correlated systems*, A. Filippetti and N. A. Spaldin, Phys. Rev. B **67**, 125109 (2003).
 29. *First principles indicators of metallicity and cation off-centricity in the IV-VI rock-salt chalcogenides of divalent Ge, Sn and Pb*, U. V. Waghmare, N. A. Spaldin, H. C. Kandpal and R. Seshadri, Phys. Rev. B **67**, 125111 (2003).

-
28. *First-principles approach to spin-orbit coupling in dilute magnetic semiconductors*, G. J. Theurich and N. A. Hill, Phys. Rev. B **66**, 115208 (2002).
 27. *Density functional studies of multiferroic magnetoelectrics*, N. A. Hill, Ann. Rev. Mat. **32**, 1 (2002).
 26. *First principles study of intrinsic defects in (Ga,Mn)As*, S. Sanvito and N. A. Hill, J. Mag. Mag. Mat. **242**, 441 (2002).
 25. *Why are there any magnetic ferroelectrics?*, N. A. Hill and A. Filippetti, J. Mag. Mag. Mat. **242**, 976 (2002).
 24. *Influence of quantum confinement on the electronic and magnetic properties of (Ga,Mn)As diluted magnetic semiconductor*, S. Sapra, D. D. Sarma, S. Sanvito and N. A. Hill, Nanoletters **2**, 605 (2002).
 23. *Coexistence of magnetism and ferroelectricity in perovskites*, A. Filippetti and N. A. Hill, Phys. Rev. B **65**, 195120 (2002).
 22. *First principles search for multiferroism in BiCrO₃*, N. A. Hill, P. Baettig and C. Daul, J. Phys. Chem. B **106**, 3383 (2002).
 21. *Density functional calculations for III-V diluted ferromagnetic semiconductors: A review*, S. Sanvito, G. J. Theurich and N. A. Hill, J. Supercon. **15**, 85 (2002).
 20. *Prediction of enhanced ferromagnetism in (Ga,Mn)As by intrinsic defect manipulation*, S. Sanvito and N. A. Hill, J. Mag. Mag. Mat. **238**, 252 (2002).
 19. *Ab-initio transport theory for digital ferromagnetic heterostructures*, S. Sanvito and N. A. Hill, Phys. Rev. Lett. **87**, 267202 (2001).
 18. *First principles study of structural, electronic and magnetic interplay in ferroelectromagnetic yttrium manganite*, A. Filippetti and N. A. Hill, J. Mag. Mag. Mat. **236**, 176 (2001).
 17. *Visualizing the role of Bi 6s “lone pairs” in the off-center distortion in ferromagnetic BiMnO₃*, R. Seshadri and N. A. Hill, Chemistry of Materials **13**, 2892 (2001).
 16. *Self-consistent treatment of spin-orbit coupling in solids using relativistic fully separable ab initio pseudopotentials*, G. J. Theurich and N. A. Hill, Phys. Rev. B **64**, 073106 (2001).
 15. *Influence of the local As antisite distribution on ferromagnetism in (Ga,Mn)As*, S. Sanvito and N. A. Hill, Appl. Phys. Lett. **78**, 3493 (2001).
 14. *First principles study of the origin and nature of ferromagnetism in (Ga,Mn)As*, S. Sanvito, P. Ordejon, N. A. Hill, Phys. Rev. B **63**, 165206 (2001).

13. *Making the Fortran to C transition: How painful is it really?*, G. J. Theurich, B. Anson, N. A. Hill and A. J. Hill, *Computing in Science and Engineering*, p.22, Jan/Feb 2001.
12. *Ground state of half-metallic zincblende MnAs*, S. Sanvito and N. A. Hill, *Phys. Rev. B* **62**, 15553 (2000).
11. *Magnetic stress as a driving force of structural distortions: The case of CrN*, A. Filippetti and N. A. Hill, *Phys. Rev. Lett.* **85**, 5166 (2000).
10. *First principles study of strain/electronic interplay in ZnO; Stress and temperature dependence of the piezoelectric constants*, N. A. Hill and U. V. Waghmare, *Phys. Rev. B* **62**, 8802 (2000).
9. *Why are there so few magnetic ferroelectrics?*, N. A. Hill, *J. Phys. Chem. B* **104**, 6694 (2000).
8. *Optical properties of Si-Ge semiconductor nano-onions*, N. A. Hill, S. Pokrant and A. J. Hill, *J. Phys. Chem. B* **103**, 3156 (1999).
7. *First principles investigation of ferromagnetism and ferroelectricity in bismuth manganite*, N. A. Hill and K. M. Rabe, *Phys. Rev. B.* **59**, 8759 (1999).
6. *Two-particle calculation of excitonic effects in semiconductor nanocrystals*, N. A. Hill and K. B. Whaley, *Chemical Physics* **210**, 117 (1996).
5. *A theoretical study of light emission from nanoscale silicon*, N. A. Hill and K. B. Whaley, *Journal of Electronic Materials* **25**, 269 (1996).
4. *Theoretical analysis of the geometries of the luminescent regions in porous silicon*, N. A. Hill and K. B. Whaley, *Appl. Phys. Lett.* **67**, 1125 (1995).
3. *Size dependence of excitons in silicon nanocrystals*, N. A. Hill and K. B. Whaley, *Phys. Rev. Lett.* **75**, 1130 (1995).
2. *A theoretical study of the influence of the surface on the electronic structure of CdSe nanoclusters*, N. A. Hill and K. B. Whaley, *J. Chem. Phys.* **100**, 2831 (1994).
1. *Electronic structure of semiconductor nanoclusters; A time-dependent theoretical approach*, N. A. Hill and K. B. Whaley, *J. Chem. Phys.* **90**, 3707 (1993).

CONFERENCE PROCEEDINGS

Computational design of a new magnetic ferroelectric, in *Magnetoelectric interaction phenomena in crystals*, N. A. Hill, Proceedings of the Fifth International Meeting on Magnetoelectric Interaction Phenomena in Crystals, Sudak, Ukraine, Kluwer Academic (2004).

First principles study of two magnetic ferroelectrics, N. A. Hill, Proceedings of the Pakistan Physical Society's 8th National Symposium on Frontiers in Physics (2000).

First principles study of multiferroic magnetoelectric manganites, N. A. Hill, Proceedings of the Aspen Workshop on Fundamental Physics of Ferroelectrics, AIP conference proceedings **535**, 372 (2000).

First principles investigation of multiferroism in perovskite manganites, N. A. Hill and K. M. Rabe, Materials Research Society Proceedings **574**, (1999).

Calculation of the electronic structure of silicon nanocrystals, N. A. Hill and K. B. Whaley, Materials Research Society Proceedings **358**, 25 (1995).

INVITED PRESENTATIONS

2021

International Conference on Advanced Materials and Devices, Jeju Island, South Korea
(Online)

*Layer and spontaneous polarizations in perovskite oxides and the influence of their
interplay on bulk and surface properties*

Berlin-Brandenburg Academy of Sciences, workshop on New Trends in Theoretical
Materials Research and Chemistry (Online)

The “Modern” Theory of Polarization 30 years on. What’s new?

Stonybrook University Materials Department Seminar (Online)

In search of electrostatic happiness

University of Warwick, Condensed Matter Physics Seminar (Online)

*From Condensed Matter to Cosmology: Studying the early universe under the mi-
croscope*

University of Geneva, Postdoc Day (Online)

Finding happiness and Saving the World through Materials Science

Trends in Magnetism, Palermo, Italy (Online)

Hidden, entangled and resonating order

MaX School on Electronic Structure Calculations, International Centre for Theoretical
Physics, Trieste (Online)

Finding happiness and saving the world with electronic structure calculations

Annual Symposium of Students in Materials Science & Engineering, Materials Research
Institute of the National Autonomous University of Mexico (Online)

Finding happiness and saving the world using Materials Science

Materials Research Society Spring Meeting (Online)

*On the happiness of ferroelectric perovskite surfaces and its role in water dissoci-
ation: The example of BiFeO₃*

Rennes Institute of Chemistry (Online)

Finding happiness and saving the world using Materials Chemistry

International Workshop on Computational Physics and Materials Science: Total Energy
and Force Methods, International Centre for Theoretical Physics, Trieste (Online)

Finding Happiness and Saving the World through Electronic-Structure Calculations

Cambridge University Chemical Society (Online)

Finding happiness and saving the world using Materials Chemistry

UBC Quantum Matter Institute, Condensed Matter Seminar (Online)
Hidden magnetoelectric multipoles in multiferroics and superconductors

2020

Workshop on Dynamic Quantum Matter and Materials, U Florida (Online)
Why hidden magnetoelectric multipoles can't stay hidden at surfaces

MARVEL NCCR Electronics Industry Day (Online)
Multiferroics beyond electric-field control of magnetism

Swiss National Science Foundation Scéance de Reflexion (Online)
Reflections on Academic Collaborations

UC Merced, Physics Colloquium (Online)
From Materials to Cosmology: Studying the early universe under the microscope

Russia Condensed Matter Colloquia (Online)
Transition-metal oxides

Cambridge University Scientific Society (Online)
New materials for a new age

Virtual Science Forum Long Range Colloquium (Online)
From Materials to Cosmology: Studying the early universe under the microscope

International Workshop on Advanced Materials, Ras al Khaimah, UAE
My Favorite Grand Challenges for Materials Chemistry: Cosmic Strings, the Higgs Boson, Dark Matter and Room-Temperature Superconductivity

Jozef Stefan Institute Colloquium, Ljubljana, Slovenia
From Materials to Cosmology: Studying the early universe under the microscope

Imperial College London, UK, Bauerman Medal Lecture
New materials for a new age

2019

Lawrence Berkeley National Lab. Distinguished Women in Science, Berkeley, CA, USA
Hidden, entangled and resonating order

Alexey Soluyanov Memorial Symposium, Zürich, Switzerland
Hidden magnetoelectric monopoles

European Research Council Scientific Seminar, Brussels, Belgium
New Materials for a New Age

Materials Research Society Fall Meeting, Boston, USA

Hidden magnetoelectric monopoles

University of Chicago, Pritzker School of Molecular Engineering Quantum Seminar, IL, USA

Hidden magnetoelectric multipoles in multiferroics and superconductors

Northwestern University, Department of Materials Science and Engineering Dorn Lecture, IL, USA

From Materials to Cosmology; Studying the early universe under the microscope

EPFL Institute of Physics Colloquium, Lausanne, Switzerland

Hidden, entangled and resonating order

Joint European Magnetic Symposia, Uppsala, Sweden (Plenary)

Hidden, entangled and resonating order

International Conference on Materials Chemistry, Birmingham, UK (Plenary)

New Materials for a New Age

Magnetism 2019, Leeds, UK (Plenary)

Hidden magnetoelectric multipoles in multiferroics and superconductors

American Physical Society March Meeting, Boston, USA

Dynamical Multiferroicity

University of Tokyo, Tokyo, Japan

From Multiferroics to Cosmology; Studying the early universe under the microscope

RIKEN, Tokyo, Japan

Hidden magnetoelectric multipoles in multiferroics and superconductors

2018

Science and Cocktails, Copenhagen, Denmark

New Materials for a New Age

Correlated Electrons in Transition-Metal Compounds: New Challenges, Dresden, Germany

Beyond Moscow in the '50s

Royal Society Fellows Research Weekend, Chicheley Hall, UK

New Materials for a New Age

Falling Walls, Berlin

Breaking the walls to the next Materials Age

International Workshop on Oxide Electronics, Les Diablerets, Switzerland

Connecting ferroelectricity and superconductivity in SrTiO₃

Leverhulme Research Centre Inaugural Symposium, U. Liverpool, UK (Keynote)

Grand challenges in Materials Chemistry

International Conference on Magnetism, San Francisco, CA (Plenary)

Hidden magnetic order in multiferroics and superconductors

The Durham Lectures, Durham University, Durham, UK

New Materials for a New Age

From Materials to Cosmology: Studying the early universe under the microscope

Hidden magnetoelectric multipoles in multiferroics and superconductors

Paul Scherrer Institute Condensed Matter Colloquium, Villigen, Switzerland

Hidden magnetoelectric multipoles in multiferroics and superconductors

Physikalische Gesellschaft Zürich, Switzerland

From Multiferroics to Cosmology; Studying the early universe under the microscope

Women's Wealth Club, Zürich, Switzerland

New Materials: Essential or Luxury?

Lise Meitner Lecture, DPG Meeting, Berlin, Germany

New Materials for a New Age

Lise Meitner Lecture, DPG Meeting, Erlangen, Germany

From Materials to Cosmology; Studying the early universe under the microscope

British Crystallographic Association Meeting, Warwick UK (Plenary)

From Multiferroics to Cosmology; Studying the early universe under the microscope

Balazs Gyorffy Colloquium, University of Bristol, UK

From Materials to Cosmology; Studying the early universe under the microscope

Gordon Research Conference on Ultrafast Phenomena in Cooperative Systems, Galveston, TX, USA

Dynamical Multiferroicity

Spanish Condensed Matter Physics Meeting, Valencia, Spain (Keynote)

From Multiferroics to Cosmology; Studying the early universe under the microscope

2017

World.Minds, Zürich, Switzerland

New Materials for a New Age

Materials Research Society Fall Meeting, Boston, USA (Mid-Career Award Talk)

Dynamical Multiferroicity

Lise Meitner Lecture, Vienna, Austria
New Materials for a New Age

Bragg Lecture, University College London, UK
From Materials to Cosmology; Studying the early universe under the microscope

Nature Conference on Ferroic Challenges and Opportunities, Xi'an, China
Dynamical Multiferroicity

MPI Quantum Matter Symposium, Berlin, Germany
Dynamical Multiferroicity

International Centre for Theoretical Physics Colloquium, Trieste, Italy
From Materials to Cosmology; Studying the early universe under the microscope

Career Development Workshop for Women in Physics, ICTP, Trieste, Italy
Multiferroics and Me

Diamond Light Source Seminar, Oxfordshire, UK
From Multiferroics to Cosmology; Studying the early universe under the microscope

Dynamic Summer Distinguished Lecture, LANL, Los Alamos, USA
From Materials to Cosmology; Studying the early universe under the microscope

Royal Society New Fellows Seminar, London, UK
Multiferroic Materials for a New Age

International Conference on Strongly Correlated Electron Systems, Prague, Czech Republic
Ferroelectricity, Multiferroicity and Superconductivity

TU Dresden Physics Colloquium, Dresden, Germany
From Materials to Cosmology; Studying the early universe under the microscope

Swedish eSciences Research Center, Stockholm, Sweden
Computing strings, from the atomic to the cosmic

International School on Oxide Electronics, Cargèse, France
Theory of multiferroics and magnetoelectrics

French Academy of Sciences (L'Oreal-UNESCO Prize Talk), Paris, France
Multiferroics: Past, present and future

Oxford University Physics Colloquium, Oxford, UK
From Materials to Cosmology; Studying the early universe under the microscope

RIKEN Symposium on Emergent Materials, Tokyo, Japan
Ferroelectricity, multiferroicity and superconductivity

2016

Materials Research Society Fall Meeting, Boston, MA, USA (Symposium X)

Multiferroics, past, present and future

European Physical Society Condensed Matter Division conference, Groningen, the Netherlands (plenary)

Multiferroics from the very small to the very big

Joint European Magnetism Symposia, Glasgow, UK (plenary)

Hidden magnetoelectric multipoles in multiferroics and superconductors

Gordon Conference on Multiferroics, Bates College, Maine, USA

The link between multiferroics, high-temperature superconductivity (and dark matter)

Hermes International Summer School, London, England

Electronic structure calculations for high-energy physics and cosmology

Lennard-Jones Center, Cambridge, England

Master Class: Ferroelectrics and phonons from first-principles

NanoGUNE Colloquium, San Sebastian, Spain

From Multiferroics to Cosmology; Studying the early universe under the microscope

Frontiers of Materials Modeling, Thomas Young Centre 10th Anniversary Symposium, London, UK

Electronic structure calculations for high-energy physics and cosmology

Physics Colloquium, University of Duisburg-Essen, Duisburg, Germany

From Multiferroics to Cosmology; Studying the early universe under the microscope

2015

Stuttgart University and Max Planck Institute Physics Colloquium, Stuttgart, Germany

From Multiferroics to Cosmology; Studying the early universe under the microscope

MRS Fall meeting, Boston MA, USA

Hidden monopolar order in magnetoelectrics and high- T_c cuprate superconductors

Electronic Properties of Modern Materials, Diamond Light Source, UK (keynote)

Hidden monopolar order in magnetoelectrics

Freiburg University Physics Colloquium, Freiburg, Germany

From Multiferroics to Cosmology; Studying the early universe under the microscope

Workshop on Oxide Electronics, Paris, France

Defect chemistry as a control parameter in oxide thin films: Insights from electronic-structure calculations

ETH Physical Chemistry Colloquium, Zürich, Switzerland

From Solid-State Chemistry to Cosmology; Studying the early universe under the microscope

Körber Prize Symposium, Hamburg, Germany

From Multiferroics to Cosmology; Studying the early universe under the microscope

Workshop on spin-lattice computations, Stockholm, Sweden

Why we would like to be able to do spin-lattice computations

Advances in Nanoscience Applications, Cambridge, UK

Magnetic monopoles and room-temperature superconductivity

TRR80 Summer School on Functionality of Correlated Materials, Chiemsee, Germany

Multiferroics

Frontiers in Advanced Materials, Bangalore, India

Hidden monopolar order in magnetoelectrics

Frontiers in Chemical Science, Weizmann Institute, Israel

From Materials Chemistry to Cosmology; Studying the early universe under the microscope

SFB Colloquium, University of Hamburg, Hamburg, Germany

Hidden monopolar order in magnetoelectrics

Advanced Materials and Nanotechnology conference, Nelson, New Zealand (keynote)

From Materials to Cosmology; Studying the early universe under the microscope

Theory of Condensed Matter Seminar, University of Cambridge, UK

From Materials to Cosmology; Studying the early universe under the microscope

Computational Nanomagnetism Seminar, KTH, Sweden

Hidden monopolar order in magnetoelectrics

2014

Royal Society of Chemistry Christmas meeting, Glasgow, UK

From Solid State Chemistry to Cosmology; Studying the early universe under the microscope

St. Andrew's University Joint Physics and Chemistry Colloquium, UK

From Materials to Cosmology; Studying the early universe under the microscope

European Spallation Source Foundation Stone Laying Ceremony, Lund, Sweden
Room temperature superconductivity and the ESS

KTH Physics Colloquium, Stockholm, Sweden
From Materials to Cosmology; Studying the early universe under the microscope

Solid State Chemistry Gordon Conference, New Hampshire, USA
Cosmic strings in multiferroics

INM Leibniz Institute for New Materials, Saarbrücken, Germany
Coupled and competing instabilities in oxide thin films: Insights from electronic-structure calculations

IBM Rüschlikon, Switzerland
From Materials to Cosmology; Studying the early universe under the microscope

Uppsala University Physics Colloquium, Sweden
From Materials to Cosmology; Studying the early universe under the microscope

Chemistry Department Seminar, U. Fribourg, Switzerland
From Materials to Cosmology; Studying the early universe under the microscope

APS March meeting, Denver, CO, USA
Hidden monopolar order in magnetoelectrics

Condensed Matter Physics Seminar, Oxford University, England
Cosmic strings in multiferroics

Tritech Consulting, Stockholm, Sweden
From Materials to Cosmology; Studying the early universe under the microscope

2013

FIRST-QS2C Workshop on Emergent Phenomena in Correlated Materials, Tokyo, Japan
Monopoles in magnetoelectrics

Seminar, Rutgers University, New Brunswick, New Jersey
Monopoles in magnetoelectrics

18th Conference of the European Theoretical Spectroscopy Facility, Luxembourg City, Luxembourg
Why I would like to able to do theoretical spectroscopy

Dynamical Properties of Solids (DyProSo) Workshop, Vienna, Austria
Cosmic strings in multiferroics

Nordita workshop on Superconductivity: The second century, Stockholm, Sweden
Ab initio studies of oxide thin films: What we can and cannot do and why

European School on Multiferroics, Wittenberg, Germany
Multiferroics in high energy physics and cosmology

U. Karlsruhe Physics Colloquium, Karlsruhe, Germany
Cosmic strings in multiferroics

U. Liège Physics Colloquium, Liège, Belgium
Cosmic strings in multiferroics

5th APCTP Workshop on Multiferroics, Singapore
Cosmic strings in multiferroics

U. Geneva Physics Colloquium, Geneva, Switzerland
Cosmic strings in multiferroics

Stanford University Applied Physics Colloquium, Stanford, CA, USA
Cosmic strings in multiferroics

Materials Research Society Spring meeting, San Francisco, CA, USA
Reversible phase transitions in multiferroics and cosmic string formation in the early universe

German Physical Society Meeting, Regensburg, Germany
Cosmic strings in multiferroics

Larmor Lecture, Queen's University, Belfast
From multiferroics to cosmology: Studying the early universe under the microscope

Workshop on Computational Physics and Materials Science: Total Energy and Force Methods, Trieste, Italy
From multiferroics to cosmology with electronic structure calculations

Edgar Lüscher Seminar, Klosters, Switzerland
Simulating cosmic string formation in a frustrated magnet

2012

MRS Fall meeting, Boston MA, USA
Coupled and competing contributions to magnetoelectric response; Insights from electronic structure theory

EPFL Materials Department Colloquium, Lausanne, Switzerland
From multiferroics to cosmology: Scaling behavior and beyond in the hexagonal manganites

CECAM Tutorial: Density functional theory: Basics, response and excitations, Zürich, Switzerland
Magnetism basics

Paul Scherrer Institute, Villigen, Switzerland

A really boring pedagogical lecture on the linear magnetoelectric effect and how to calculate it

Nordic Institute for Theoretical Physics, Stockholm, Sweden

From multiferroics to cosmology: Scaling behavior and beyond in the hexagonal manganites

Royal Society Discussion Meeting – Magnetoelectric phenomena and devices

A really boring pedagogical lecture on the linear magnetoelectric effect and how to calculate it

CSCS User Day, Lugano, Switzerland

From transition metal oxides to cosmic strings

CCCP5 Summer School, Cardiff, U.K.

From transition metal oxides to cosmic strings

IFW, Dresden, Germany

Revisiting the hexagonal manganites: From multiferroics to cosmology (and how electronic structure calculations can help)

Uppsala University Materials Seminar, Sweden

From multiferroics to cosmology (and how electronic structure calculations can help)

University of Frankfurt Physics Colloquium, Germany

From multiferroics to cosmology (and how electronic structure calculations can help)

Ecole Polytechnique, Physics Department, Paris, France

From multiferroics to cosmology (and how electronic structure calculations can help)

Nature conference on Frontiers in Electronic Materials, Aachen Germany

Revisiting the hexagonal manganites; From multiferroic interfaces to cosmic strings

WE Hereus Seminar on New Routes to Single-Phase Multiferroics, Bad Honnef, Germany

Revisiting the hexagonal manganites; From multiferroic interfaces to cosmic strings

Paul Scherrer Institute Microscopy and Magnetism Meeting, Lungern, Switzerland

Designer tunable interfaces in complex oxides

Orange County Conference on Spintronics, Bangalore, India

Revisiting the hexagonal manganites; From multiferroic interfaces to cosmic strings

Indian Institute of Science, Bangalore, India

Revisiting the hexagonal manganites; From multiferroic interfaces to cosmic strings

Jawaharlal Nehru Center for Advanced Scientific Research, Bangalore, India

Revisiting the hexagonal manganites; From multiferroic interfaces to cosmic strings

Fifth European School on Multiferroics, Ascona, Switzerland

Multiferroics – classification and how to find a room temperature one

2011

Thomas Young Centre, London, England, Colloquium

Recent advances in electronic structure theory; From complex oxides to cosmic strings

International Workshop on Functionality from Heterostructures, Obergurgl, Austria

Revisiting the hexagonal manganites; From multiferroics to cosmic strings

NSF Distinguished Lectureship in Mathematical and Physical Sciences, VA, USA

Using density functional theory to design new materials: From magnetoelectronics to a theory of everything

Swiss Association of Computational Chemists Meeting, Bern, Switzerland (Plenary)

Using density functional theory to design new materials: From magnetoelectronics to a theory of everything

ETH Zürich Physics Colloquium

Using density functional theory to design new materials: From magnetoelectronics to a theory of everything

Workshop on Multifunctional Oxides and Minerals, Uppsala, Sweden

Multiferroics: Whence, why and whither?

DPG Meeting, Dresden, Germany

Using density functional theory to design new materials: From magnetoelectronics to a theory of everything

Vienna Computational Materials Workshop, Vienna, Austria

Using density functional theory to design new materials: From magnetoelectronics to a theory of everything

EMPA Colloquium, Dübendorf, Switzerland

Using density functional theory to design new materials: From magnetoelectronics to a theory of everything

Paul Scherrer Institute Colloquium, Villigen, Switzerland

Using density functional theory to design new materials: From magnetoelectronics to a theory of everything

2010

Gotham Metro meeting, New York Academy of Sciences

Using density functional theory to design new materials: From magnetoelectronics to a theory of everything

Physics Colloquium, UC San Diego, CA

Using density functional theory to design new materials: From magnetoelectronics to a theory of everything

Physics Colloquium, Gran Sasso National Laboratory, L'Aquila, Italy

Using density functional theory to design new materials: From magnetoelectronics to a theory of everything

Multiscale Modeling of Materials Conference, Freiburg, Germany

Using density functional theory to design new materials: From magnetoelectronics to a theory of everything

Physics Colloquium, UC Merced, CA

Using density functional theory to design new materials: From magnetoelectronics to a theory of everything

Indo-Sweden Workshop, Uppsala, Sweden

What can first-principles calculations contribute to understanding the toroidal moment in bulk periodic solids

Electroceramics XII, Trondheim, Norway (Keynote)

Using density functional theory to design new materials; Magnetoelectronics and the origin of the universe

Materials Department Seminar, ETH, Zurich, Switzerland

Using density functional theory to design new materials; Magnetoelectronics and the origin of the universe

CECAM Workshop on First-Principles Calculations for Magnetoelectrics, Lausanne, Switzerland

What can first-principles calculations contribute to understanding the toroidal moment in bulk periodic solids

Magnetoelectrics; Whence, why and wither?

MPG FKF Seminar, Stuttgart, Germany

Oxide/Oxide interfaces from first principles; Design and understanding

Joint IFW/PKS Colloquium, Dresden, Germany

Using density functional theory to design new materials; Magnetoelectronics and the origin of the universe

Materials Department Seminar, KTH, Stockholm, Sweden

Using density functional theory to design new materials; Magnetoelectronics and the origin of the universe

U. Halle Physics Colloquium, Halle, Germany

Using density functional theory to design new materials; Magnetoelectronics and the origin of the universe

Uppsala University, Complex Systems Seminar, Uppsala, Sweden

Using density functional theory to design new materials. From nanoelectronics to the origin of the universe

APS March meeting, Portland, OR

A theorist's-eye view of multiferroics (McGroddy Prize Talk)

Fundamental Physics of Ferroelectrics, Aspen, CO

The role of first-principles calculations in understanding and designing multiferroics

Kavli Institute of Theoretical Physics, Santa Barbara, CA

Whither (or wither) multiferroics?

2009

MRS Fall meeting, Boston MA

Oxide/Oxide interfaces from First Principles; Design and Understanding

Yale University MRSEC Colloquium, New Haven, CT

Using density functional theory to design new materials; Magnetoelectronics and the origin of the universe

Argonne National Labs., Chicago, IL

Using density functional theory to design new materials; Magnetoelectronics and the origin of the universe

European School on Multiferroics, Groningen, Netherlands

Multiferroics; Recent history, current excitement and future directions

Zernike Insitute, U. Groningen, Netherlands

Using density functional theory to design new materials; Magnetoelectronics and the origin of the universe

Mott Meeting, Santa Barbara, CA

Use of first-principles computations in designing and understanding oxide/oxide interfaces

International Conference on Magnetism, Karlsruhe, Germany (Semi-Plenary)

Novel magnetism at strongly correlated interfaces

Summer School on Materials Modeling from First Principles, Santa Barbara, CA
(Keynote)

Using density functional theory to design new materials

MRS Spring meeting, San Francisco, CA

Picozzi-inspired routes to novel magnetoelectrics

Materials Department Colloquium, Iowa State University, Ames, IA

How do we use computational methods to design new materials?

2008

ICMR/ICMS Winter School on Novel Oxide and Carbon Materials, Bangalore, India

Why oxides are interesting and hard to calculate (and why these are related)

MRS Fall meeting, Boston, MA

New routes to electric field control of magnetism

UCSB Physics Graduate Student Seminar, Santa Barbara, CA

How do we use computational methods to design new materials?

Colloquium, CIMAV National Lab., Chihuahua, Mexico

Recent progress in single phase multiferroics

NanoFeronics-2008, Jülich, Germany

Recent progress in single phase multiferroics

Workshop on Ordering Phenomena in Transition Metal Oxides, Augsburg, Germany

Towards a microscopic theory of toroidal moments in periodic crystals

Physics Department Colloquium, Harvey Mudd College, Claremont, CA

How do we use computational methods to design new materials?

Gordon Conference on Correlated Electrons, Biddeford, ME

New routes to electric field control of magnetism

Ehrenfest Colloquium, Lorentz Institute, Leiden, Netherlands

New routes to electric field control of magnetism

European MRS meeting, Strasbourg, France

New routes to electric field control of magnetism

Materials Colloquium, U. Washington, Seattle

New routes to electric field control of magnetism

Physics Colloquium, U. Frankfurt

New routes to electric field control of magnetism

NordinSpin 08, Gimo Herrgard, Sweden

New routes to electric field control of magnetism

APS meeting, New Orleans, LA

Towards a microscopic theory of toroidal moments in bulk, crystalline solids

TMS meeting, New Orleans, LA

Exploiting oxide interfaces to generate new functionalities

Indo-Japan Workshop on New directions in ferroics and multiferroics, Kolkata, India

Progress and prospects in magnetoelectrics and multiferroics

Materials Colloquium, UC Santa Barbara

New routes to electric-field control of magnetism

ISIS Colloquium, UC Irvine

New routes to electric-field control of magnetism

2007

Angstrom Laboratory, Uppsala University, Sweden

Progress and prospects in multiferroics and magnetoelectrics

Jawaharlal Nehru Center for Advanced Scientific Research, India

Multiferroics and magnetoelectrics

CNSI seminar, UCLA

Design of new magnetoelectrics and multiferroics

Zernike Institute Colloquium, U. Groningen, Netherlands

Progress and prospects in multiferroics and magnetoelectrics

The National Academies, Irvine, CA

Grand challenges in oxides research

Northwestern University, Materials Colloquium

Progress and prospects in multiferroics

International Conference on Electroceramics, Arusha, Tanzania (**Plenary**)

Progress and prospects in multiferroics

Pan American Advanced Study Institute on Electronic States and Excitations on Nanostructures, Zacatecas, Mexico

Multiferroics and magnetoelectrics

International Symposium on Correlated Electron Systems, Akihabara, Japan

Alternative mechanisms for the magnetoelectric effect

International Symposium on Integrated Ferroelectrics, Bordeaux, France
First principles calculations for metal-ferroelectric interfaces

University of Bonn, Physics Colloquium
Computational design of contra-indicated multifunctional materials

MRS Spring meeting, San Francisco, CA
Ab initio calculations of complex oxide interfaces

iDFT07, Laguna Beach, CA
Electric fields in DFT calculations; problems and solutions

EMMA MURI Review, Berkeley, CA
The dielectric dead layer in nanoscale capacitors: existence, origin, mitigation and exploitation

Lawrence Berkeley Labs. Seminar
Progress and prospects in multiferroics

Washington University at St. Louis, Physical Chemistry Seminar
Computational design of contra-indicated multifunctional materials

Caltech, Materials Colloquium
Computational design of contra-indicated multifunctional materials

Rensselaer Polytechnic Institute, Materials Colloquium
Computational design of contra-indicated multifunctional materials

IBM Almaden, Seminar
Progress and prospects in multiferroics: A theorist's perspective

UC Berkeley, Miller Institute Seminar
First-principles design of contra-indicated multifunctional materials

Physics and Chemistry of Semiconductor Interfaces, Salt Lake City, UT
Ab initio calculations for complex oxide interfaces

2006

Materials Research Society Fall Meeting, Boston, MA
Progress in thin film multiferroics
First principles calculations for nanoscale capacitors

California Condensed Matter Theory Meeting, Santa Barbara, CA
Progress and prospects in multiferroics: A theorist's perspective

University of Central Florida, Physics Colloquium
Computational design of contra-indicated multifunctional materials

Florida State University, Materials Colloquium

Computational design of contra-indicated multifunctional materials

Magnetic Nanostructures Gordon Conference, Oxford, UK

Progress and prospects in multiferroics: A theorist's perspective

Solid State Chemistry Gordon Conference, New London, NH

Computational design of contra-indicated multifunctional materials

Workshop on Computational Materials Theory, Bangalore, India

Computational design of contra-indicated multifunctional materials

Summer School on Electronic Structure Methods, Bangalore, India

Introduction to functional materials

International Symposium on Structure-Property Relationships in Solid State Materials,
Bordeaux, France

Progress in magnetoelectric multiferroics

UC Santa Barbara, Physical Chemistry Seminar

Computational design of contra-indicated multifunctional materials

University of Toronto, Canada, Condensed Matter Physics Seminar

Why are there so few magnetic ferroelectrics?

Frontiers in Inorganic Materials Chemistry, Santa Barbara, CA

Contra-indicated multifunctional materials: Intelligent design, creation and evolution

Oak Ridge National Labs., Oak Ridge, TN, Center for Nanomaterials Colloquium

Computational design of new multiferroics

Louisiana State University, Baton Rouge, LA, Physics Colloquium

Why are there so few magnetic ferroelectrics?

2005

Stanford University, CA, Materials Colloquium

Why are there so few magnetic ferroelectrics?

Workshop on Oxide Electronics, Cape Cod, MA

Progress in magnetoelectric multiferroics

Ψ_k Conference, Schwabisch Gmünd, Germany

Density functional studies of multiferroics

Fritz-Haber Institute, Berlin, Germany

Computational design of contra-indicated multifunctional materials

American Chemical Society National Meeting, Washington, DC

Computational design of contraindicated multifunctional materials

Telluride Workshop on Physics of Novel Oxides, Telluride, CO

Density functional studies of multiferroics

Czech Academy of Sciences, Prague, Czech Republic

Computational design of new multiferroics

National Academy of Sciences Frontiers of Science Symposium, Irvine, CA

Computational design of multifunctional materials

UC Santa Cruz, Chemistry Dept. Inorganic Seminar

Computational design of new multifunctional materials

International Workshop on Prospects in Magnetic Oxides, Fontevraud, France

Density functional studies of multiferroics

APS March meeting, Los Angeles, CA

Density functional studies of multiferroics

Conference on Fundamental Physics of Ferroelectrics, Williamsburg, VA

Recent developments in multiferroics

Materials Research Outreach Symposium, UCSB

Designing new multifunctional materials and violating some laws of physics and chemistry

Science and Engineering Council of Santa Barbara

Chemical design of new multifunctional materials

2004

Los Alamos National Labs.

Can an electric field reverse a spontaneous magnetization?

MRS Fall meeting, Boston, MA

Computational design of multifunctional oxides.

Origin of ferromagnetism in novel spintronic oxides

Workshop on Predictive Capabilities for Strongly-Correlated Systems, Oak Ridge, TN

Comparison between different functionals for transition metal oxides

American Vacuum Society International Symposium, Anaheim, CA

Computational design of multifunctional electronic materials

NSF Workshop on Materials Theory, Arlington, VA

Ab initio design of new multifunctional materials

UC Berkeley, Solid State Physics Seminar

Computational design of new multifunctional materials

UCSB/Oxford Workshop on Advanced Materials, Oxford, UK

Computational design of new multifunctional materials

Inorganic Materials in the UC system, UCSB

A theorist's-eye view of MRL collaborations: How to persuade people to grow your materials

UCLA, Mechanical Engineering Dept. Seminar

Computational design of new multifunctional materials

NSF/ITR Workshop, UIUC, IL

Computational design of new multifunctional materials

ABINIT Electronic Structure Workshop, Paris, France

Organizing software development for computational design of new materials

University of Houston, Chemistry Dept. Colloquium

Computational design of new multifunctional materials

Columbia University, Physics Dept. Seminar

Computational design of new multifunctional materials

Rutgers University, Chemistry Dept. Colloquium

Computational design of new multifunctional materials

NSF/EC Workshop on Computational Materials, San Francisco, CA

Computational design of new spintronic materials

TMS Annual Meeting, Charlotte, NC

Computational design of new spintronic materials

TMS Annual Meeting, NSF-sponsored panel on Future of Metals, Charlotte, NC

Designer approaches to multifunctional metals

UCSB/MPI Workshop on Advanced Materials, Santa Barbara, CA

Computational design of new multifunctional materials

2003

University of Washington, Seattle, Materials Dept. Colloquium

Why are there so few magnetic ferroelectrics?

Fall Meeting of the American Ceramic Society, Oakland, CA

Computational design of new magnetic ferroelectrics

Magnetoelectric Interaction Phenomena in Crystals V, Sudak, Ukraine
Why are there so few magnetic ferroelectrics?

Chemistry of Electronic Materials Gordon Conference, New London, CT
Computational design of multiferroics

University of Lancaster, Physics Dept. Colloquium
New materials for nanospintronics

Cambridge University, Theory of Condensed Matter Seminar
Who I am, where I come from, what I do and where I am going

Accelrys Inc., Cambridge, U.K.
Computational design of new materials

Cambridge University, Materials Dept. Seminar
Why are there so few magnetic ferroelectrics?

TU Dresden, Chemistry Dept. Seminar
Computational design of multiferroics

University of Lancaster, Physics Dept. Seminar
Self-interaction corrections and why we need them (sometimes)

Cambridge University, Physics Dept. Seminar
Why are there so few magnetic ferroelectrics?

Cambridge University, Earth Sciences Seminar
Self-interaction corrections and why we need them (sometimes)

Trinity College, Dublin, Physics Dept. Colloquium
Computational design of new magnetic materials

Condensed Matter and Materials Physics Conference, Belfast, Ireland
A new mechanism for ferroelectricity and a new ferroelectric with an old mechanism

International Symposium on Integrated Ferroelectrics , Colorado Springs, CO
Computational design of new multiferroics

Conference on Fundamental Physics of Ferroelectrics, Williamsburg, VA
A new mechanism for ferroelectricity and a new ferroelectric with an old mechanism

Michigan State University, Physics Dept. Seminar
Computational design of new magnetic materials

2002

University of Michigan, Ann Arbor, Materials Dept. Colloquium
Computational design of new magnetic materials

Solid State Chemistry Gordon Conference, New London, NH
Computational design of new spintronic materials

UC San Diego, Physics Dept. Seminar
New materials for nanospintronics

CNRS Workshop on Advanced Materials, Paris, France
New materials for nanospintronics

MRS Spring meeting, San Francisco, CA
Computational design of new multiferroic perovskites

APS March meeting, Indianapolis, IN
Computational design of new multiferroic materials

National Science Foundation IGERT P.I. Workshop, Washington, DC
Interdisciplinary graduate education at UCSB: Mentoring and Diversity

Hughes Research Labs., Malibu, CA
Pushing the limits of electronic structure theory; Can we design new spintronic materials?

2001

California State University, Northridge
Why are there so few magnetic ferroelectrics?

EPFL-ETHZ-UCSB-WIS Workshop on Advanced Materials, Cret-Bérard, Switzerland
Why are there so few magnetic ferroelectrics?

EPFL, Switzerland
Why are there any magnetic ferroelectrics?

University of Fribourg, Switzerland
First principles prediction of diferroism in BiCrO_3

CNRS, Grenoble, France
Why are there so few magnetic ferroelectrics?

Joint European Magnetism Symposium, Grenoble, France
Why are there any magnetic ferroelectrics?

Los Alamos National Lab.
Why are there so few magnetic ferroelectrics?

Spintronics 2001, Georgetown
Pushing the limits of electronic structure theory; can we design new spintronic materials?

ICTP/UCSB/TWAS workshop, Trieste, Italy

Pushing the limits of electronic structure theory; Can we design new spintronic materials?

Corning Incorporated

Spintronics Materials Research at UCSB

ACS Spring meeting, San Diego, CA

Design of new multiferroic materials using computational solid state chemistry

San Diego State University, Physics Dept. Colloquium

Why are there so few magnetic ferroelectrics?

2000

Pakistan Physical Society's 8th National Symposium on Frontiers in Physics, Lahore

First principles study of two magnetic ferroelectrics

IIT Delhi, Dept. of Chemistry Seminar

Why are there so few magnetic ferroelectrics?

Jawaharlal Nehru Center for Advanced Scientific Research

Why are there so few magnetic ferroelectrics?

Jawaharlal Nehru Center for Advanced Scientific Research

New materials for Nanospintronics

Indian Institute of Science, Solid State Chemistry Unit

Why are there so few magnetic ferroelectrics?

Materials Research Outreach Symposium, UCSB

Why are there so few magnetic ferroelectrics?

Aspen Center for Physics

Why are there so few magnetic ferroelectrics?

1999

QUEST Seminar, UCSB

Multiferroism and magnetoresistance in manganites - a new class of materials for magnetic data storage?

UCLA, Dept. of Chemistry Seminar

Multiferroism and magnetoresistance in manganites - a new class of materials for magnetic data storage?

UCSB-MRL/IMN-CNRS Workshop, Nantes, France

Multiferroism and magnetoresistance in manganites - a new class of materials for magnetic data storage?

UCSB-MRL/CSIRO/KAIST Workshop on Advanced Materials

Multiferroism and magnetoresistance in manganites - a new class of materials for magnetic data storage?

1998

UC Berkeley, Materials Dept. Colloquium

Multiferroism and magnetoresistance in manganites - new materials for magnetic data storage?

UC San Diego, Solid State Physics Seminar

First principles investigation of ferromagnetic ferroelectric BiMnO_3 - a new perspective on the perovskite manganites

UC Irvine, Solid State Physics Seminar

First principles investigation of ferromagnetic ferroelectric BiMnO_3 - a new perspective on the perovskite manganites

1997

Cambridge University, England, Physics Dept. Seminar

First principles study of ferromagnetic ferroelectrics

Fachbereich Physikalische Chemie der Phillips-Universität Marburg, Germany

First-principles design of new materials for magnetic data storage

NIST Center for Theoretical and Computational Materials Science

Bismuth manganite - the ferromagnetic ferroelectric perovskite

1996

University of California at Santa Barbara, Materials Department

Calculating the electronic properties of semiconductor nanostructures

1995

AT&T Bell Laboratories

Calculating the electronic properties of semiconductor nanostructures

College of William & Mary, Applied Sciences Dept. Seminar

Calculating the electronic properties of semiconductor nanostructures

California Institute of Technology, Applied Physics Seminar

Calculating the electronic properties of nanometer-sized semiconductor structures