Four Requests from an Experimentalist to Bold Theorists

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In this talk I make four requests from the perspective of an experimentalist whose life has been changed by his positive interactions with theorists over the past dozen years. For two long decades I was a struggling fisherman until I saw the light and began to talk to and, more importantly, to listen to bold theorists who provided maps of where to find big fish. These bold theorists made materials-specific predictions of where to put the atoms to get new or enhanced properties—and many times they were right. Today all of my research, which involves the heteroepitaxial growth and characterization of oxide thin films by reactive molecular-beam epitaxy (MBE), utilizes a "materials-by-design" approach to discover materials with properties superior to any known. Working together with theorists, we have unleashed unparalleled properties—those of hidden ground states—by exploiting large strains in concert with the ability to precisely control dimensionality and stabilize metastable phases in epitaxial oxide heterostructures.[1] For example, materials that are not ferroelectric or ferromagnetic in their unstrained state can be transmuted into materials that are both at the same time.[2] Similarly, we exploit epitaxial engineering to tune the band structure of the correlated oxides with the perovskite structure as well as their two-dimensional counterparts. The band structure is revealed by high-resolution angle-resolved photoemission (ARPES) on pristine as-grown surfaces of these complex oxides made possible by a direct ultra-high vacuum connection between MBE and ARPES systems.[3-10] Our work demonstrates the possibility of utilizing strain engineering as a disorder-free means to manipulate emergent properties and many-body interactions in correlated materials. The approach that I describe is now available to users like you through a new national user facility sponsored by the National Science Foundation called the *Platform for the Accelerated Realization, Analysis, and Discovery of Interface Materials* (PARADIM).[11]

My four requests of the next generation of bold theorists—those of you in this theory winter school—are:

- Please do *not* pollute the literature with predictions on impossible materials
- Please do consider the limits of synthesis
- Please do use the new NSF-MIP National User Facilities (PARADIM[11] + 2DCC[12])
- Please do tell me first if you predict a materials-specific embodiment of a room-temperature superconductor!

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1 D.G. Schlom, L.Q. Chen, C.J. Fennie, V. Gopalan, D.A. Muller, X.Q. Pan, R. Ramesh, and R. Uecker, "Elastic Strain Engineering of Ferroic Oxides," *MRS Bulletin* **39** (2014) 118–130.

2 J.H. Lee, L. Fang, E. Vlahos, X. Ke, Y.W. Jung, L.F. Kourkoutis, J-W. Kim, P.J. Ryan, T. Heeg, M. Roeckerath, V. Goian, M. Bernhagen, R. Uecker, P.C. Hammel, K.M. Rabe, S. Kamba, J. Schubert, J.W. Freeland, D.A. Muller, C.J. Fennie, P. Schiffer, V. Gopalan, E. Johnston-Halperin, and D.G. Schlom, "A Strong Ferroelectric Ferromagnet Created by means of Spin-Lattice Coupling," *Nature* **466** (2010) 954–958.

[3] E.J. Monkman, C. Adamo, J.A. Mundy, D.E. Shai, J.W. Harter, D. Shen, B. Burganov, D.A. Muller, D.G. Schlom, and K.M. Shen, "Quantum Many-Body Interactions in Digital Oxide Superlattices," *Nature Materials* **11** (2012) 855–859. See also the accompanying News and Views, J. M. Rondinelli and S. J. May, "Oxide Interfaces: Instrumental Insights," *Nature Materials* **11** (2012) 833–834.

[4] D.E. Shai, A.J. Melville, J.W. Harter, E.J. Monkman, D.W. Shen, A. Schmehl, D.G. Schlom, and K.M. Shen, "Temperature Dependence of the Electronic Structure and Fermi-Surface Reconstruction of $Eu_{1-x}Gd_xO$ through the Ferromagnetic Metal-Insulator Transition," *Physical Review Letters* **108** (2012) 267003.

[5] J.W. Harter, L. Maritato, D.E. Shai, E.J. Monkman, Y.F. Nie, D.G. Schlom, and K.M. Shen, "Nodeless Superconducting Phase Arising from a Strong (π,π) Antiferromagnetic Phase in the Infinite-Layer Electron- Doped $Sr_{1-x}La_xCuO_2$ Compound," *Physical Review Letters* **109** (2012) 267001.

[6] D.E. Shai, C. Adamo, D.W. Shen, C.M. Brooks, J.W. Harter, E.J. Monkman, B. Burganov, D.G. Schlom, and K.M. Shen, "Quasiparticle Mass Enhancement and Temperature Dependence of the Electronic Structure of Ferromagnetic $SrRuO_3$ Thin Films," *Physical Review Letters* **110** (2013) 087004.

[7] P.D.C. King, H.I. Wei, Y.F. Nie, M. Uchida, C. Adamo, S. Zhu, X. He, I. Božović, D.G. Schlom, and K.M. Shen, "Atomic-Scale Control of Competing Electronic Phases in Ultrathin $LaNiO_3$," *Nature Nanotechnology* **9** (2014) 443-447.

[8] Y.F. Nie, P.D.C. King, C.H. Kim, M. Uchida, H.I. Wei, B.D. Faeth, J.P. Ruf, J.P.C. Ruff, L. Xie, X.Q. Pan, C.J. Fennie, D.G. Schlom, and K.M. Shen, "Interplay of Spin-Orbit Interactions, Dimensionality, and Octahedral Rotations in Semimetallic $SrIrO_3$," *Physical Review Letters* **114** (2015) 016401.

[9] Y.F. Nie, D. Di Sante, S. Chatterjee, P.D.C. King, M. Uchida, S. Ciuchi, D.G. Schlom, and K.M. Shen, "Formation and Observation of a Quasi-Two-Dimensional d_{xy} Electron Liquid in Epitaxially Stabilized $Sr_{2-x}La_xTiO_4$ Thin Films," *Physical Review Letters* **115** (2015) 096405.

[10] B. Burganov, C. Adamo, A. Mulder, M. Uchida, P.D.C. King, J.W. Harter, D.E. Shai, A.S. Gibbs, A.P. Mackenzie, R. Uecker, M. Bruetzam, M.R. Beasley, C.J. Fennie, D.G. Schlom, and K.M. Shen, "Strain Control of Fermiology and Many-Body Interactions in Two-Dimensional Ruthenates," *Physical Review Letters* **116** (2016) 197003.

[11] See www.PARADIM.org

[12] See www.mri.psu.edu/mip