

## ALEXIE M. KOLPAK

Department of Mechanical Engineering  
77 Massachusetts Ave  
Cambridge, MA 02139

Building 3, Rm 158  
phone: (617) 324-6768  
email: kolpak@mit.edu

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### EDUCATION

B.A. in Biochemistry, University of Pennsylvania, Philadelphia, PA. 2002  
M.S. in Chemistry, University of Pennsylvania, Philadelphia, PA. 2002  
Ph.D. in Physical Chemistry, University of Pennsylvania, Philadelphia, PA. 2007

### CURRENT POSITION

**Assistant Professor, Mechanical Engineering, MIT.** 2012-present  
*Rockwell International Chair*

### RESEARCH EXPERIENCE

**Postdoctoral Associate, Materials Science, MIT.** 2010-2012  
*Advisor: Prof. Jeffrey C. Grossman.*

- First principles-based atomic-scale design of novel materials for solar energy harvesting and storage (focus on solar thermal fuels, organic and inorganic photovoltaics).
- Development of and participation in ARPA-E-funded collaboration to make predicted solar thermal fuels and develop devices/applications.

**Postdoctoral Associate, Applied Physics, Yale University.** 2007-2010  
*Advisor: Prof. Sohrab Ismail-Beigi.*

- Collaborated with experimental colleagues to predict atomic structure, multi-scale properties, and growth kinetics of epitaxial SrTiO<sub>3</sub>/Si and BaO/Si heterostructures.
- Used *ab initio* computations to design a novel class of atomic-layer thick ferroelectrics.
- Predicted electronic, magnetic, and defect properties of LaAlO<sub>3</sub>/SrTiO<sub>3</sub> heterostructures.

**Research Assistant, Chemistry, University of Pennsylvania.** 2003-2007  
*Advisor: Prof. Andrew M. Rappe.*

- Predicted effects of interface chemistry on ferroelectricity in ultrathin film ferroelectric oxide capacitors and designed a dynamically tunable metal/ferroelectric catalyst.
- Determined phase diagram of the BaTiO<sub>3</sub> surface with experimental colleagues.
- Predicted adsorbate-induced ferroelectricity in ultrathin PbTiO<sub>3</sub> films and BaTiO<sub>3</sub> nanowires and demonstrated in collaboration with experimental colleagues.

### RESEARCH INTERESTS

Computational modeling of fundamental processes coupled with atomic-scale materials design and experimental collaboration to address energy and environmental challenges, particularly in:

#### Catalysis.

- Dynamically tunable catalysts for efficient CO<sub>2</sub> capture and conversion.
- Polar nanostructures for water splitting and other photocatalytic reactions.
- New methods for *ab initio* prediction of realistic atomic structure and properties of oxide/solvent interfaces.

#### Photovoltaics and electronics.

- Multiferroic and opto-electronic materials.
- Nanostructured hybrid organic/inorganic photovoltaics.
- Effects of atomic structure and stoichiometry on band alignment and charge transfer across metal/oxide and oxide/semiconductor interfaces.

## HONORS

- University of Pennsylvania Vagelos Scholar. 1998–2002
- Phi Beta Kappa. 2002
- Hypercube Chemistry Award for undergraduate research. 2002
- Atofina Fellowship for graduate research. 2005
- Invited Talks:
  - Navy Research Labs, Washington, DC. March 2007
  - Department of Applied Physics, Yale University, New Haven, CT. April 2007
  - Argonne National Labs, Argonne, IL. May 2007
  - American Chemical Society National Meeting, Washington, DC. August 2007
  - Villa Conference on Oxide Heterostructures, Orlando, FL. October 2008
  - Materials Research Society Spring Meeting, San Francisco, CA. April 2010
  - Department of Materials Science and Engineering, MIT, Cambridge, MA. May 2010
  - Center for Simulational Physics Workshop, Athens, GA. February 2011
  - Department of Materials Science, Cornell University, Ithaca, NY. April 2011
  - Department of Physics, Washington University, St. Louis, MO. October 2011
  - Energy Harvesting & Storage USA 2011, Boston, MA. November 2011
  - Department of Solid Mechanics, Brown University, Providence, RI. December 2011
  - Department of Chemical and Biological Engineering, UIUC, Urbana, IL. February 2012
  - Department of Materials Science, Yale University, New Haven, CT. February 2012
  - Department of Mechanical Engineering, MIT, Cambridge, MA. March 2012
  - Department of Physics, UC Berkeley, Berkeley, CA. March 2012
  - TMS Spring Meeting, Orlando, FL. March 2012
  - April APS Meeting, Atlanta, GA. April 2012
  - International Workshop on Computational Electronics, Madison, WI. May 2012

## PUBLICATIONS

### Refereed Journals:

- B. Kolb and A. M. Kolpak, “Ultrafast bandgap oscillations in iron pyrite,” *Phys. Rev. B* **88**, 235208 (2013).
- A. M. Kolpak and J. C. Grossman, “Hybrid chromophore/template nanostructures: a customizable platform material for solar energy storage and conversion,” *J. Chem. Phys.* **138**, 034303 (2013).
- K. F. Garrity, A. M. Kolpak, and S. Ismail-Beigi, “Ferroelectric surface chemistry: a first-principles study of CO<sub>2</sub> on PbTiO<sub>3</sub>,” *Phys. Rev. B* **88**, 045401 (2013).
- K. F. Garrity, A. M. Kolpak, and S. Ismail-Beigi, “Growth and interfacial properties of epitaxial oxides on semiconductors: *ab initio* insights,” *J. Mater. Science* **47**, 7417 (2012).
- A. M. Kolpak and S. Ismail-Beigi, “Interface structure and film polarization in epitaxial SrTiO<sub>3</sub>/Si(001),” *Phys. Rev. B* **85**, 195318 (2012).
- M. A. Mendez Polanco, I. Grinberg, A. M. Kolpak, S. V. Levchenko, C. Pynn, and A. M. Rappe, “Stabilization of highly polarized PbTiO<sub>3</sub> nanoscale capacitors due to in-plane symmetry breaking at the interface,” *Phys. Rev. B* **85**, 214107 (2012).
- A. M. Kolpak and J. C. Grossman, “Azobenzene-Functionalized Carbon Nanotubes As High-Energy Density Solar Thermal Fuels,” *Nano Letters*, **11**, 3156 (2011).
  - News articles in *MIT News*, *PhysicsWorld*, *Wired* (July/Aug. 2011).
  - Highlighted in the *MRS Bulletin* (Sept. 2011).
- A. M. Kolpak and S. Ismail-Beigi, “Thermodynamic stability and growth kinetics of epitaxial SrTiO<sub>3</sub> on silicon,” *Phys. Rev. B* **83**, 165318 (2011).
  - Selected as an Editor’s Suggestion in *Phys. Rev. B*.
- A. M. Kolpak, F. J. Walker, J. W. Reiner, Y. Segal, D. Su, M. S. Sawicki, C. C. Broadbridge, Z.

Zhang, Y. Zhu, C. H. Ahn, and S. Ismail-Beigi, "Inhibition of ferroelectricity in Si/SrTiO<sub>3</sub> due to intrinsic interface effects," *Phys. Rev. Lett.* **105**, 217601 (2010).

- Selected as an Editor's Suggestion in *Phys. Rev. Lett.*
- Highlighted in *Physics* (physics.aps.org) (Nov. 17, 2010).
- H. Chen, A. M. Kolpak, and S. Ismail-Beigi, "Electronic and magnetic properties of the SrTiO<sub>3</sub>/LaAlO<sub>3</sub> interface from first-principles," *Adv. Mater.* **22**, 28812899 (2010).
- K. Garrity, A. M. Kolpak, S. Ismail-Beigi, and E. A. Altman, "Chemistry of ferroelectric surfaces," *Adv. Mater.* **22**, 2969 (2010).
- J. W. Reiner, A. M. Kolpak, Y. Segal, K. F. Garrity, S. Ismail-Beigi, C.H. Ahn, and F. J. Walker, "Crystalline oxides on semiconductors," *Adv. Mater.* **22**, 29192938 (2010).
- D. P. Kumah, J. W. Reiner, Y. Segal, A. M. Kolpak, Z. Zhang, D. Su, Y. Zhu, M. S. Sawicki, C. Broadbridge, C. H. Ahn, and F. J. Walker, "The atomic structure and polarization of strained SrTiO<sub>3</sub>/Si," *Appl. Phys. Lett.* **97**, 251902 (2010).
- H. Chen, A. M. Kolpak, and S. Ismail-Beigi, "A first-principles study of LaAlO<sub>3</sub>/SrTiO<sub>3</sub> heterointerfaces and their variants," *Phys. Rev. B* **82**, 085430 (2010).
- Y. Segal, J. W. Reiner, A. M. Kolpak, Z. Zhang, S. Ismail-Beigi, C. H. Ahn, and F. J. Walker, "Atomic structure of the epitaxial BaO/Si(001) interface," *Phys. Rev. Lett.* **102**, 116101 (2009).
- R.-V. Wang, D. D. Fong, F. Jiang, S. K. Strieffer, P. H. Fuoss, C. Thompson, J. A. Eastman, A. M. Kolpak, A. M. Rappe, K. Latifi, and G. B. Stephenson, "Reversible chemical switching of a ferroelectric film," *Phys. Rev. Lett.* **102**, 047601 (2009).
  - Selected as an Editor's Suggestion in *Phys. Rev. Lett.*
  - Highlighted as a *Physics* Viewpoint (physics.aps.org) (Jan. 26, 2009)
- H. Chen, A. M. Kolpak, and S. Ismail-Beigi, "Fundamental asymmetry in interfacial electronic reconstruction between insulating oxides: An *ab initio* study," *Phys. Rev. B* **79**, 161402 (2009).
- Li, M. He, J. Garra, A. M. Kolpak, A. M. Rappe, D. A. Bonnelli, and J. Vohs, "Direct *in situ* determination of the polarization dependence of adsorption on ferroelectric surfaces," *Nature Materials* **7**, 473 (2008).
- S. H. Shah, P. D. Bristowe, A. M. Kolpak, and A. M. Rappe. "First principles study of three-component SrTiO<sub>3</sub>/BaTiO<sub>3</sub>/PbTiO<sub>3</sub> ferroelectric superlattices," *J. Mater. Sci.* **43**, 3750 (2008).
- A. M. Kolpak, I. Grinberg, and A. M. Rappe, "Polarization effects on the surface chemistry of PbTiO<sub>3</sub>-supported Pt films," *Phys. Rev. Lett.* **98**, 166101 (2007).
- A. M. Kolpak, D. Li, R. Shao, D. A. Bonnelli, and A. M. Rappe, "Evolution of the structure and thermodynamic stability of the BaTiO<sub>3</sub>(001) surface," *Phys. Rev. Lett.* **101**, 036102 (2007).
- J. E. Spanier, A. M. Kolpak, J. J. Urban, I. Grinberg, O. Y. Lian, W. S. Yun, A. M. Rappe, and H. Park, "Ferroelectric phase transition in individual single-crystalline BaTiO<sub>3</sub> nanowires," *Nano Letters* **6**, 735 (2006).
- D. Fong, A. M. Kolpak, J. A. Eastman, S. K. Strieffer, P. H. Fuoss, G. B. Stephenson, C. Thompson, D. M. Kim, K. J. Choi, C. B. Eom, I. Grinberg, and A. M. Rappe, "Stabilization of monodomain polarization in ultrathin PbTiO<sub>3</sub> films," *Phys. Rev. Lett.* **96**, 127601 (2006).
- A. M. Kolpak, N. Sai and A. M. Rappe, "Short-circuit boundary conditions in ferroelectric PbTiO<sub>3</sub> thin films," *Phys. Rev. B* **74**, 054112 (2006).
- V. R. Cooper, A. M. Kolpak, Y. Yourdshahyan, and A. M. Rappe, "Supported metal electronic structure: Implications for molecular adsorption," *Phys. Rev. B* **72**, 081409-1-4 (2005).
- N. Sai, A. M. Kolpak, and A. M. Rappe, "Ferroelectricity in ultrathin perovskite films," *Phys. Rev. B* **72**, 020101 (2005).

Work submitted for publication:

- T. J. Kucharski, J. O. Zheng, N. Ferralis, A. M. Kolpak, D. G. Nocera, and J. C. Grossman,

“Packing heat: Templating photoswitches for high energy density solar thermal fuels,” under review, *Nature Chemistry*, (2013).

- A. M. Kolpak and S. Ismail-Beigi, “Functional monolayers on semiconductors,” submitted to *Phys. Rev. Lett.*

*Conference Proceedings and Book Chapters:*

- V. R. Cooper, A. M. Kolpak, Y. Yourdshahyan, and A. M. Rappe, Oxide-supported metal thin-film catalysts: The how and why, *Nanotechnology in Catalysis, Volume 3*, B. Zhou, R. Raja, S. Han, and G. A. Somorjai, (Eds.), Springer, New York, 2006.
- Y. Yourdshahyan, V. R. Cooper, A. M. Kolpak, and A. M. Rappe, “Catalytic behavior at the nanoscale: CO adsorption on Al<sub>2</sub>O<sub>3</sub>-supported Pt clusters,” *Proc. SPIE* **5223**, 223 (2004).

*Patents:*

- A. Buonassisi, J. C. Grossman, N. Tabet, E. Johlin, A. M. Kolpak, C. Simmons, D. Strubbe, and T. Kirkpatrick, “Enhanced charge collecting a-Si:H solar cell,” (pending).
- A. M. Kolpak and J. C. Grossman, “Azobenzene functionalized carbon nanotubes and other templated photoswitch molecules for high energy density solar thermal fuels,” (pending).
- A. M. Kolpak, F. J. Walker, J. W. Reiner, C. H. Ahn, and S. Ismail-Beigi, “Ferroelectric devices including a layer having two or more stable configurations,” (pending).
- A. M. Rappe and A. M. Kolpak, “Tunable ferroelectric supported catalysts and methods and use thereof,” (pending).
- A. M. Rappe, Na Sai, and A. M. Kolpak, “Ferroelectric ultrathin perovskite films,” Patent No. US 7,768,050 B2, Aug. 3, 2010.