Peter Doak

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Education

University of California, Berkeley	Chemistry	Ph.D., 2014
Brown University	Modern Culture and Media	BA, 1996

Research Interests

1. Abinitio based mesoscale modeling:
   - Model the formation of molecular surface layers on surfaces capturing emergent phe- nomena such as long-range order and edge reconstruction in n-part systems.
   - Using parameters derived from first principals calculations such as DFT predict the structure of new molecules on surfaces.
2. Excited states on surfaces:
   - How do one and two quasiparticle states change in the vicinity of a screening surface?
   - What beyond DFT theory is required to get good answers?
   - What physically motivated approximations can we make to calculate these energies from simpler model systems?
   - What is the effect of long-range order of surface layers on excited states?

Professional Experience

2014-Present Postdoctoral Researcher, Center for Nanophase Materials Sciences
2008-2014 Graduate Student Research Assistant, Lawrence Berkeley National Lab

Publications

- Cedeno, D., Krawicz, A., Doak, P., Yu, M., Neaton, J. B. & Moore, G. F. Using molecular design to control the performance of hydrogen-producing polymer-brush-modified photocathodes. *J. Phys. Chem. Lett.* **5,** 3222–3226 (2014).
- Li, Y., Doak, P., Kronik, L., Neaton, J. B. & Natelson, D. Voltage tuning of vibrational mode energies in single-molecule junctions. *Proc. Natl. Acad. Sci. U. S. A.* **111,** 1282–7 (2014).
- Ugeda, M. M., Yu, M., Bradley, A. J., Doak, P., Liu, W., Moore, G. F., Sharp, I. D., Tilley, T. D., Neaton, J. B. & Crommie, M. F. Adsorption and stability of π-bonded ethylene on GaP(110). *J. Phys. Chem. C* **117,** 26091–26096 (2013).
- Sharifzadeh, S., Tamblyn, I., Doak, P., Darancet, P. T. & Neaton, J. B. Quantitative molecular orbital energies within a G0W0 approximation. *Eur. Phys. J. B* **85,** (2012).
- Malen, J. a., Doak, P., Baheti, K., Don Tilley, T., Segalman, R. a. & Majumdar, A. Identifying the length dependence of orbital alignment and contact coupling in molecular heterojunctions. *Nano Lett.* **9,** 1164–1169 (2009).
- Malen, J. a., Doak, P., Baheti, K., Tilley, T. D., Majumdar, A. & Segalman, R. a. The nature of transport variations in molecular heterojunction electronics. *Nano Lett.* **9,** 3406–3412 (2009).
- Baheti, K., Malen, J. A., Doak, P., Reddy, P., Jang, S. Y., Tilley, T. D., Majumdar, A. & Segalman, R. A. Probing the chemistry of molecular heterojunctions using thermoelectricity. *Nano Lett.* **8,** 715–719 (2008).
- Dukovic, G., Balaz, M., Doak, P., Berova, N. D., Zheng, M., Mclean, R. S. & Brus, L. E. Racemic single-walled carbon nanotubes exhibit circular dichroism when wrapped with DNA. *J. Am. Chem. Soc.* **128,** 9004–9005 (2006).

Graduate and Postdoctoral Advisors

Ph.D. Advisor: Prof. Jeffrey B. Neaton (University of California, Berkeley)
Postdoctoral Advisor: Panchapakesan Ganesh (ORNL)