

Stanford



Evan Reed

Associate Professor of Materials Science and Engineering

CONTACT INFORMATION

- **Administrator**

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Bio

BIO

We are engaged in theory and modeling of materials at the atomic scale. Our recent work has two primary directions:

1. Monolayer and few layer materials (i.e. graphene, MoS₂) for electronics, NEMS, and energy applications.
2. Materials at conditions of high temperature, electromagnetic fields, and pressures, including dynamic or shock compression.

Recent research topics include piezoelectricity and phase change effects in monolayer materials. Past topics include THz radiation generation, energetic materials, and photonic crystals. We develop and utilize computational tools (molecular dynamics statistical methods, electronic structure, materials informatics approaches, etc.) and interact closely with experimentalists.

ACADEMIC APPOINTMENTS

- Associate Professor, Materials Science and Engineering

HONORS AND AWARDS

- ONR Young Investigator Program Award (YIP), Office of Naval Research (2015)
- NSF Career Award, NSF (2014)
- Young Faculty Award, DARPA (2012)
- Robert Noyce Faculty Scholar, Stanford University School of Engineering (2010-2013)
- Ernest O. Lawrence Postdoctoral Fellow, Lawrence Livermore National Laboratory (2004 - 2007)

PROGRAM AFFILIATIONS

- Stanford SystemX Alliance

PROFESSIONAL EDUCATION

- BS, Caltech, Applied Physics (1998)
- PhD, MIT, Physics (2003)

Teaching

COURSES

2018-19

- Atom-based computational methods for materials: MATSCI 331 (Win)
- Atomic Arrangements in Solids: MATSCI 193, MATSCI 203 (Aut)
- Nanoscale Materials Physics Computation Laboratory: MATSCI 165, MATSCI 175 (Spr)

2017-18

- Atom-based computational methods for materials: MATSCI 331 (Win)
- Atomic Arrangements in Solids: MATSCI 193, MATSCI 203 (Aut)
- Nanoscale Materials Physics Computation Laboratory: MATSCI 165, MATSCI 175 (Spr)

2016-17

- Atom-based computational methods for materials: MATSCI 331 (Spr)
- Atomic Arrangements in Solids: MATSCI 193, MATSCI 203 (Aut)

2015-16

- Atom-based computational methods for materials: MATSCI 331 (Spr)
- Atomic Arrangements in Solids: MATSCI 193, MATSCI 203 (Aut)
- Materials Science Colloquium: MATSCI 230 (Spr)
- Nanoscale Materials Physics Computation Laboratory: MATSCI 165, MATSCI 175 (Win)

STANFORD ADVISEES

Doctoral Dissertation Reader (AC)

Kristopher Brown, Isha Datye, Minda Deng, Alex Gabourie, Varun Harbola, Anjali Patel, Marc Zajac, Dante Zakhidov

Postdoctoral Faculty Sponsor

Rodrigo Freitas

Doctoral Dissertation Advisor (AC)

Evan Antoniuk, Gowoon Cheon, Vincent Dufour Decieux, Aditi Krishnapriyan, Brandi Ransom, Michael Tang, Yanbing Zhu

Orals Evaluator

Rohit Prasanna

Doctoral Dissertation Co-Advisor (AC)

Jaime Avilés Acosta

Master's Program Advisor

Yunzhi Liu, Wenjie Ma, Wei Ren, Chandrahaas Vadali, Xiang Wu, Yumeng Yue

Postdoctoral Research Mentor

Rodrigo Freitas

Doctoral (Program)

Jesus Guardado, Aditi Krishnapriyan, Brandi Ransom, Michael Tang

Publications

PUBLICATIONS

- **Screening billions of candidates for solid lithium-ion conductors: A transfer learning approach for small data.** *The Journal of chemical physics*
Cubuk, E. D., Sendek, A. D., Reed, E. J.
2019; 150 (21): 214701
- **Transferable Kinetic Monte Carlo Models with Thousands of Reactions Learned from Molecular Dynamics Simulations.** *The journal of physical chemistry. A*
Chen, E., Yang, Q., Dufour-Decieux, V., Sing-Long, C. A., Freitas, R., Reed, E. J.
2019
- **Machine Learning-Assisted Discovery of Solid Li-Ion Conducting Materials** *CHEMISTRY OF MATERIALS*
Sendek, A. D., Cubuk, E. D., Antoniuk, E. R., Cheon, G., Cui, Y., Reed, E. J.
2019; 31 (2): 342–52
- **ODE integration schemes for plane-wave real-time time-dependent density functional theory.** *The Journal of chemical physics*
Rehn, D. A., Shen, Y., Buchholz, M. E., Dubey, M., Namburu, R., Reed, E. J.
2019; 150 (1): 014101
- **New Assembly-Free Bulk Layered Inorganic Vertical Heterostructures with Infrared and Optical Bandgaps** *NANO LETTERS*
Antoniuk, E. R., Cheon, G., Krishnapriyan, A., Rehn, D. A., Zhou, Y., Reed, E. J.
2019; 19 (1): 142–49
- **Revealing the Spectrum of Unknown Layered Materials with Superhuman Predictive Abilities** *JOURNAL OF PHYSICAL CHEMISTRY LETTERS*
Cheon, G., Cubuk, E. D., Antoniuk, E. R., Blumberg, L., Goldberger, J. E., Reed, E. J.
2018; 9 (24): 6967–72
- **Refrigeration in 2D: Electrostaticaloric effect in monolayer materials** *PHYSICAL REVIEW MATERIALS*
Rehn, D. A., Li, Y., Reed, E. J.
2018; 2 (11)
- **Microscopic Origins of the Variability of Water Contact Angle with Adsorbed Contaminants on Layered Materials** *JOURNAL OF PHYSICAL CHEMISTRY C*
Zhou, Y., Reed, E. J.
2018; 122 (32): 18520–27
- **Metallic Metal-Organic Frameworks Predicted by the Combination of Machine Learning Methods and Ab Initio Calculations** *JOURNAL OF PHYSICAL CHEMISTRY LETTERS*
He, Y., Cubuk, E. D., Allendorf, M. D., Reed, E. J.
2018; 9 (16): 4562–69
- **The potential for fast van der Waals computations for layered materials using a Lifshitz model** *2D MATERIALS*
Zhou, Y., Pellouchoud, L. A., Reed, E. J.
2017; 4 (2)
- **Data Mining for New Two- and One-Dimensional Weakly Bonded Solids and Lattice-Commensurate Heterostructures.** *Nano letters*
Cheon, G., Duerloo, K. N., Sendek, A. D., Porter, C., Chen, Y., Reed, E. J.
2017
- **Holistic computational structure screening of more than 12 000 candidates for solid lithium-ion conductor materials** *ENERGY & ENVIRONMENTAL SCIENCE*
Sendek, A. D., Yang, Q., Cubuk, E. D., Duerloo, K. N., Cui, Y., Reed, E. J.
2017; 10 (1): 306-320
- **Learning reduced kinetic Monte Carlo models of complex chemistry from molecular dynamics.** *Chemical science*
Yang, Q., Sing-Long, C. A., Reed, E. J.
2017; 8 (8): 5781–96

- **Quantum Nuclear Effects in Stishovite Crystallization in Shock-Compressed Fused Silica** *JOURNAL OF PHYSICAL CHEMISTRY C*
Shen, Y., Reed, E. J.
2016; 120 (31): 17759-17766
- **Structural Phase Transitions by Design in Monolayer Alloys.** *ACS nano*
Duerloo, K. N., Reed, E. J.
2016; 10 (1): 289-297
- **Structural semiconductor-to-semimetal phase transition in two-dimensional materials induced by electrostatic gating.** *Nature communications*
Li, Y., Duerloo, K. N., Wauson, K., Reed, E. J.
2016; 7: 10671-?
- **Nanosecond homogeneous nucleation and crystal growth in shock-compressed SiO₂** *NATURE MATERIALS*
Shen, Y., Jester, S. B., Qi, T., Reed, E. J.
2016; 15 (1): 60-?
- **Piezoelectricity: Now in two dimensions.** *Nature nanotechnology*
Reed, E. J.
2015; 10 (2): 106-107
- **Strain engineering in monolayer materials using patterned adatom adsorption.** *Nano letters*
Li, Y., Duerloo, K. N., Reed, E. J.
2014; 14 (8): 4299-4305
- **Structural phase transitions in two-dimensional Mo- and W-dichalcogenide monolayers.** *Nature communications*
Duerloo, K. N., Li, Y., Reed, E. J.
2014; 5: 4214-?
- **Flexural Electromechanical Coupling: A Nanoscale Emergent Property of Boron Nitride Bilayers** *NANO LETTERS*
Duerloo, K. N., Reed, E. J.
2013; 13 (4): 1681-1686
- **Simulations of Shocked Methane Including Self-Consistent Semiclassical Quantum Nuclear Effects** *JOURNAL OF PHYSICAL CHEMISTRY A*
Qi, T., Reed, E. J.
2012; 116 (42): 10451-10459
- **Intrinsic Piezoelectricity in Two-Dimensional Materials** *JOURNAL OF PHYSICAL CHEMISTRY LETTERS*
Duerloo, K. N., Ong, M. T., Reed, E. J.
2012; 3 (19): 2871-2876
- **Ultrafast Detonation of Hydrazoic Acid (HN₃)** *PHYSICAL REVIEW LETTERS*
Reed, E. J., Rodriguez, A. W., Manaa, M. R., Fried, L. E., Tarver, C. M.
2012; 109 (3)
- **Engineered Piezoelectricity in Graphene** *ACS NANO*
Ong, M. T., Reed, E. J.
2012; 6 (2): 1387-1394
- **Electron-Ion Coupling in Shocked Energetic Materials** *JOURNAL OF PHYSICAL CHEMISTRY C*
Reed, E. J.
2012; 116 (3): 2205-2211
- **Observation of terahertz radiation coherently generated by acoustic waves.** *Nature Physics*
Reed, E. J., Armstrong, M., R. et al.
2009; 5: 285-288
- **Theoretical potential for low energy consumption phase change memory utilizing electrostatically-induced structural phase transitions in 2D materials** *NPJ COMPUTATIONAL MATERIALS*
Rehn, D. A., Li, Y., Pop, E., Reed, E. J.
2018; 4

- **COMPUTATIONAL MATERIALS SCIENCE Two-dimensional tellurium** *NATURE*
Reed, E. J.
2017; 552 (7683): 1–2
- **Structural phase transition in monolayer MoTe2 driven by electrostatic doping** *NATURE*
Wang, Y., Xiao, J., Zhu, H., Li, Y., Alsaid, Y., Fong, K., Zhou, Y., Wang, S., Shi, W., Wang, Y., Zettl, A., Reed, E. J., Zhang, et al
2017; 550 (7677): 487+
- **Statistical learning of kinetic Monte Carlo models of high temperature chemistry from molecular dynamics**
Yang, Q., Sing-Long, C., Chen, E., Reed, E.
AMER CHEMICAL SOC.2017
- **Hundreds of new two- and one-dimensional weakly bonded solids and lattice-commensurate heterostructures via data mining**
Reed, E., Sendek, A., Duerloo, K., Porter, C., Chen, Y., Reed, E.
AMER CHEMICAL SOC.2017
- **Films.** *ACS nano*
Empante, T. A., Zhou, Y., Klee, V., Nguyen, A. E., Lu, I., Valentin, M. D., Naghibi Alvillar, S. A., Preciado, E., Berges, A. J., Merida, C. S., Gomez, M., Bobek, S., Isarraraz, et al
2017; 11 (1): 900-905
- **Ultrafast electronic and structural response of monolayer MoS2 under intense photoexcitation conditions.** *ACS nano*
Mannebach, E. M., Duerloo, K. N., Pellouchoud, L. A., Sher, M., Nah, S., Kuo, Y., Yu, Y., Marshall, A. F., Cao, L., Reed, E. J., Lindenberg, A. M.
2014; 8 (10): 10734-10742