# On Final Projects

- **What? Anything you like**
- **Written report + presentation**
- **Either *Programming*, *Critical Review* or *Proposal***

# Paper Abstract Format

## Picosecond amorphization of $SiO_2$ stishovite under tension

**Masaaki Misawa,[1,2] Emina Ryuo,[2] Kimiko Yoshida,[3] Rajiv K. Kalia,[1] Aiichiro Nakano,[1]* Norimasa Nishiyama,[4] Fuyuki Shimojo,[2] Priya Vashishta,[1] Fumihiro Wakai[3]**

*Sci. Adv*. **3**, e1602339 ('17)

***(1) Problem*: *(1a)*** It is extremely difficult to realize two conflicting properties — high hardness and toughness — in one material. Nano-polycrystalline stishovite, recently synthesized from Earth-abundant silica glass, proved to be a super-hard, ultra-tough material, which could provide sustainable supply of high-performance ceramics. ***(1b)*** **However, its toughening mechanism remains elusive.** ***(2) Finding*:** Our quantum molecular dynamics simulations show that stishovite amorphizes rapidly on the order of picosecond under tension in front of a crack tip. **We find a displacive amorphization mechanism** that only involves short-distance collective motions of atoms, thereby facilitating the rapid transformation. The two-step amorphization pathway involves an intermediate state akin to experimentally suggested "high-density glass polymorphs", before eventually transforming to normal glass. The rapid amorphization can catch up with, screen, and self-heal a fast moving crack. ***(3) So What*?** **This new concept of fast amorphization toughening likely operates in other pressure-synthesized hard solids.**

**Tell your own narrative of history & place your work within!**

# Paper Abstract Format (2)

**Towards Dynamic Simulations of Materials on Quantum Computers**

Lindsay Bassman *et al.*, *Phys. Rev. B* **101**, 184305 ('20)

***(1) Problem*: *(1a)*** With the recent experimental realization of quantum supremacy on a very specific problem, search is now on for the use of quantum computers for nontrivial scientific applications. A highly anticipated application is as a universal simulator of quantum many-body systems, as was conjectured by Richard Feynman in the 1980s and later elaborated by Seth Lloyd. The last decade has witnessed the growing success of quantum computing for simulating *static* properties of quantum systems, *i.e.*, the ground state energy of small molecules. ***(1b)*** **However, it remains a challenge to simulate quantum many-body *dynamics* on current-to-near-future noisy intermediate-scale quantum (NISQ) computers.** ***(2) Finding*:** **Here, we demonstrate successful simulation of nontrivial quantum dynamics on publicly available NISQ computers,** namely, IBM's Q16 Melbourne quantum processor and Rigetti's Aspen quantum processor. The compelling scientific problem is ultrafast control of emergent magnetism by THz radiation in an atomically-thin two-dimensional material. ***(3) So What*?** To liberate these newly available NISQ computers for broader scientific use, we also provide the full code and step-by-step tutorials for performing such simulations on each quantum processor. As such, **this work lays a foundation for the promising study of a wide variety of quantum dynamics on near-future quantum computers,** including dynamic localization of Floquet states and topological protection of qubits in noisy environments.

**Problem funnel: Narrow down to the specific problem you solved!**

# Punch-Kick Writing

articulate_

WHAT WE DO + | HOW WE WORK | ABOUT US | BLOG | RESOURCES | CONTACT US

## So what = kicker

HOW TO WRITE

## Want to write well? Open with a punch, close with a kick

There are two words that every writer needs to know: lede and kicke.r A 'lede' is the punchy opening sentence of an article. A 'kicker' is the last. If you can get them right, you can lift your writing to a whole new level.

https://www.articulatemarketing.com/blog

# Lede: Diamonds in Sky

**Since Ross proposed that there might be 'diamonds in the sky' in 1981 (ref. 1), the idea of significant quantities of pure carbon existing in giant planets such as Uranus and Neptune has gained both experimental[2] and theoretical[3] support.**

J. H. Eggert *et al*., *Nat. Phys*. **6**, 40 ('10)

Shimamura *et al*., *Nano Lett*. **14**, 4090 ('14)

## Rihanna Lyrics

**"Diamonds"**

Shine bright like a diamond
Shine bright like a diamond

Find light in the beautiful sea
I choose to be happy
You and I, you and I
We're like diamonds in the sky

***Astrochemistry*:**
**Space origin of life materials**

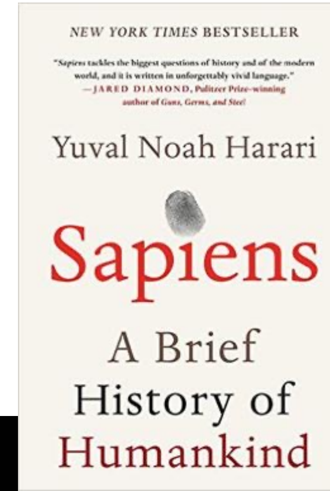
"Molecular dynamics simulations of dielectric breakdown of lunar regolith: implications for water ice formation on lunar surface," Z. Huang *et al*., *Geophys. Res. Lett.* 48, e2020GL091681 ('21)

# Winning Pattern in Science: Story

## Why → So what → Now what

“Now what” by John Hopfield (*Princeton*) Nobel physics ’24
https://pni.princeton.edu/sites/g/files/toruqf321/files/documents/John%20Hopfield%20Now%20What%203_0.pdf

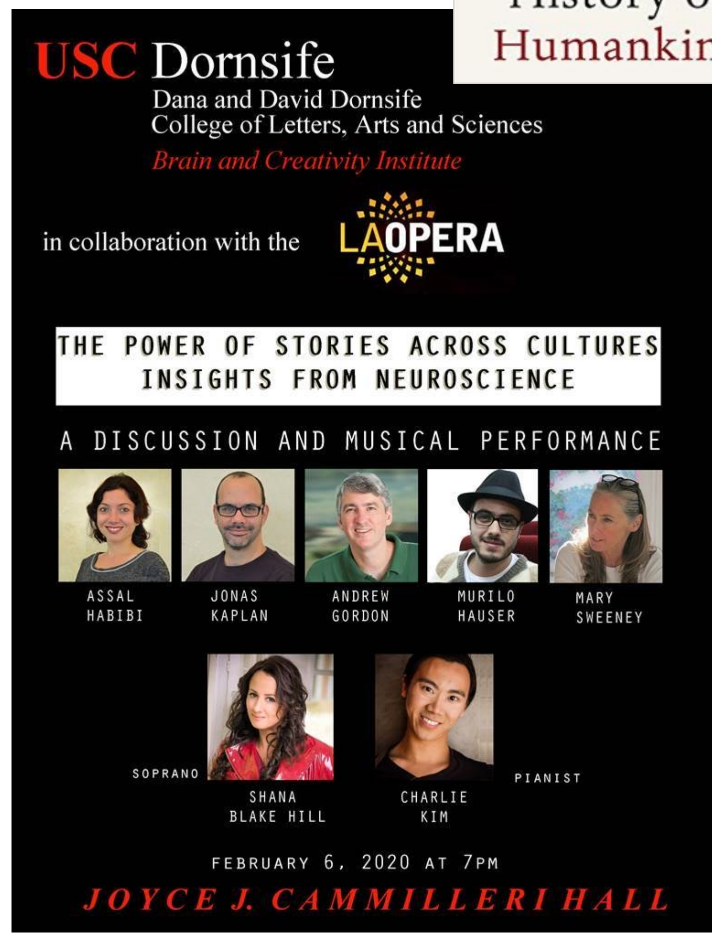
**Cognitive revolution: ~70,000 BCE, Sapiens evolved imagination & fictive language**




## It’s all telling a story!

**“I concluded some time ago that the distinguishing characteristic of human intelligence is our story competence. We tell stories, we listen to stories, and we make up new stories by blending old ones together. That’s really what education is all about, if you think about it…I think sharing the stories, the opinions, the asides, and understanding how a person solved a particular problem, what they were thinking of when they did that, what they were motivated by, etc. is just as, and probably more, important than teaching the actual skills.”**

“Open with a promise, close with a joke”
by Patrick Winston (*MIT*)
http://www.ocw-openmatters.org/2016/07/19/open-with-a-promise-close-with-a-joke/



# Neno’s Ten Questions

1. What is the main goal of your work?
2. What are the tangible benefits?
3. What are the technical problems that make that goal difficult to achieve? (*i.e*., why hasn’t this been done already?)
4. What are the main elements of your approach?
5. How does your approach handle the technical problems that have prevented progress in the past? (*i.e*., what makes you think you can do it when no one else could before?)
6. What are the unique, novel, and/or critical technologies developed in your approach?
7. What are the potential spin-offs or other applications of your work?
8. How can progress be measured? (*i.e*., how can anyone tell if/when you’ve succeeded?)
9. What have you accomplished thus far?
10. What is your schedule for the work remaining?

“Answer all before you shall be allowed to take a qualifying exam.”

Prof. Nenad Medviovic (*USC*)

# Manage Your Research with Paper

## Whitesides' Group: Writing a Paper**

By *George M. Whitesides** *Adv. Mater*. **16**, 1375 ('04)

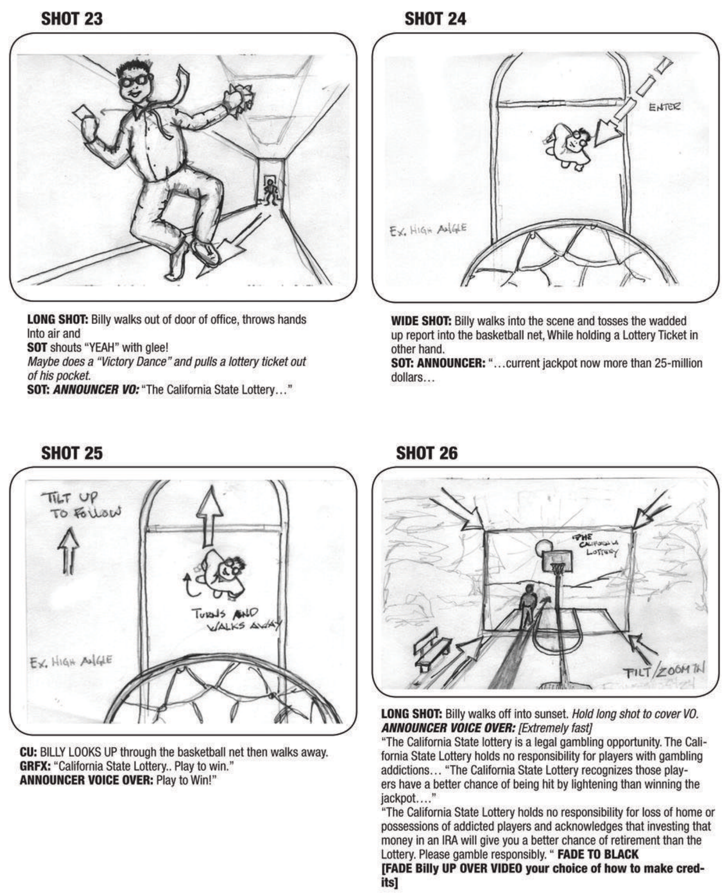
### 1. What is a Scientific Paper?

https://aiichironakano.github.io/phys516/Whitesides-WritingPaper-AdvMater04.pdf

A paper is an organized description of hypotheses, data and conclusions, intended to instruct the reader. Papers are a central part of research. If your research does not generate papers, it might just as well not have been done. "Interesting and unpublished" is equivalent to "non-existent".

Realize that your objective in research is to formulate and test hypotheses, to draw conclusions from these tests, and to teach these conclusions to others. Your objective is not to "collect data".

A paper is not just an archival device for storing a completed research program; it is also a structure for *planning* your research in progress. If you clearly understand the purpose and form of a paper, it can be immensely useful to you in *organizing* and conducting your research. A good outline for the paper is also a good plan for the research program. You should write and rewrite these plans/outlines throughout the course of the research. At the beginning, you will have mostly plan; at the end, mostly outline. The continuous effort to understand, analyze, summarize, and reformulate hypotheses on paper will be immensely more efficient for you than a process in which you collect data and only start to organize them when their collection is "complete".




*cf*. Cinema storyboard

***Do It for Your Final!***

# Team Project

- **Who did what? Team efforts are encouraged with the condition that the role of each team member is clearly delineated in the final-project report.**

*Nature Geoscience* **2**, 62 - 66 (2009)
Published online: 7 December 2008 | doi:10.1038/ngeo383

**Subject Category:** Geochemistry

## Biomolecule formation by oceanic impacts on early Earth

Yoshihiro Furukawa[1], Toshimori Sekine[2], Masahiro Oba[3], Takeshi Kakegawa[1] & Hiromoto Nakazawa[2]

## Author contributions

H.N. proposed the impact synthesis hypothesis and conducted this study. Y.F. and T.S. carried out the shock recovery experiments. Y.F. extracted organic compounds and analysed amines and amino acids using LC–MS. M.O. and Y.F. analysed carboxylic acids using GC–MS. Y.F. and H.N. prepared an earlier manuscript. All authors discussed and prepared the final manuscript.

# A Final Team

*International Journal of Computational Science*
1992-6669 (Print) 1992-6677 (Online) © Global Information Publisher
2007, Vol. 1, No. 4, 407-421

**ParaViz: A Spatially Decomposed Parallel Visualization Algorithm Using Hierarchical Visibility Ordering**

Cheng Zhang[1], Scott Callaghan[2], Thomas Jordan[2], Rajiv K. Kalia[1],
Aiichiro Nakano[1*], Priya Vashishta[1]

**material science**
***molecular dynamics***
***parallel***

**computer science**
***visualization***
***parallel***

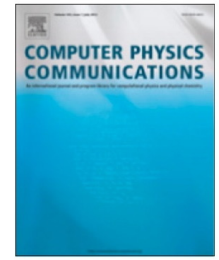
# Another Final Team

Computer Physics Communications 207 (2016) 186–192

Contents lists available at ScienceDirect

Computer Physics Communications

journal homepage: www.elsevier.com/locate/cpc




## Parallel implementation of geometrical shock dynamics for two dimensional converging shock waves

CrossMark

Shi Qiu, Kuang Liu, Veronica Eliasson*

*Aerospace and Mechanical Engineering, University of Southern California, Los Angeles, CA 90089-1191, USA*

**mechanical engineering**
***shock physics***

**computer science**
***parallel***

Computer Physics Communications homepage

# Multi-Class Project

APPLIED PHYSICS LETTERS **100**, 163108 (2012)

## Critical dimensions of highly lattice mismatched semiconductor nanowires grown in strain-releasing configurations

Suzana Sburlan,[1] P. Daniel Dapkus,[1,2] and Aiichiro Nakano[2,3]
[1]*Compound Semiconductor Laboratory, Department of Electrical Engineering, Electrophysics, University of Southern California, Los Angeles, California 90089-0242, USA*
[2]*Center for Energy Nanoscience, University of Southern California, Los Angeles, California 90089-0243, USA*
[3]*Collaboratory for Advanced Computing and Simulations, Department of Computer Science, University of Southern California, Los Angeles, California 90089-0242, USA*

JOURNAL OF APPLIED PHYSICS **111**, 054907 (2012)

## Effect of substrate strain on critical dimensions of highly lattice mismatched defect-free nanorods

Suzana Sburlan,[1,a)] Aiichiro Nakano,[2,3] and P. Daniel Dapkus[1,3]
[1]*Compound Semiconductor Laboratory, Department of Electrical Engineering, Electrophysics, University of Southern California, Los Angeles, California 90089-0243, USA*
[2]*Collaboratory for Advanced Computing and Simulations, Department of Computer Science, University of Southern California, Los Angeles, California 90089-0242, USA*
[3]*Center for Energy Nanoscience, University of Southern California, Los Angeles, California 90089-0243, USA*

**$O(N)$ Lanczos eigensolver (PHYS516) → parallelization (CSCI596/653)**

# Multi-Class Project (2)

Computer Physics Communications 219 (2017) 246–254

Contents lists available at ScienceDirect

Computer Physics Communications

journal homepage: www.elsevier.com/locate/cpc

## A derivation and scalable implementation of the synchronous parallel kinetic Monte Carlo method for simulating long-time dynamics

Hye Suk Byun [a], Mohamed Y. El-Naggar [a,b,c], Rajiv K. Kalia [a,d,e,f], Aiichiro Nakano [a,b,d,e,f,*], Priya Vashishta [a,d,e,f]

[a] Department of Physics & Astronomy, University of Southern California, Los Angeles, CA 90089-0242, USA
[b] Department of Biological Sciences, University of Southern California, Los Angeles, CA 90089-0242, USA
[c] Department of Chemistry, University of Southern California, Los Angeles, CA 90089-0242, USA
[d] Department of Computer Science, University of Southern California, Los Angeles, CA 90089-0242, USA
[e] Department of Chemical Engineering & Materials Science, University of Southern California, Los Angeles, CA 90089-0242, USA
[f] Collaboratory for Advanced Computing and Simulations, University of Southern California, Los Angeles, CA 90089-0242, USA

**Kinetic Monte Carlo (PHYS516) → parallelization (CSCI596/653)**

# More Class Projects (1)

Computer Physics Communications 239 (2019) 265–271
Contents lists available at ScienceDirect
Computer Physics Communications
journal homepage: www.elsevier.com/locate/cpc

PAR$^2$: Parallel Random Walk Particle Tracking Method for solute transport in porous media

Calogero B. Rizzo[a,*], Aiichiro Nakano[b], Felipe P.J. de Barros[a]

Computer Physics Communications 244 (2019) 324–328
Contents lists available at ScienceDirect
Computer Physics Communications
journal homepage: www.elsevier.com/locate/cpc

WaterAlignment: Identification of displaced water molecules in molecular docking using Jonker and Volgenant shortest path augmentation for linear assignment

Dab Brill[c,e,*], Jason B. Giles[e], Ian S. Haworth[e], Aiichiro Nakano[a,b,c,d,f]

Computational Materials Science 173 (2020) 109429
Contents lists available at ScienceDirect
Computational Materials Science
journal homepage: www.elsevier.com/locate/commatsci

Boltzmann machine modeling of layered $MoS_2$ synthesis on a quantum annealer

Jeremy Liu[a,b], Ankith Mohan[a], Rajiv K. Kalia[c], Aiichiro Nakano[c], Ken-ichi Nomura[c,*], Priya Vashishta[c], Ke-Thia Yao[a]

buildings
*Buildings* **9**, 44 (2019)
MDPI
*Article*

Adaptive Kinetic Architecture and Collective Behavior: A Dynamic Analysis for Emergency Evacuation

Angella Johnson[1,*], Size Zheng[2], Aiichiro Nakano[3], Goetz Schierle[1] and Joon-Ho Choi[1]

Computer Physics Communications 247 (2020) 106873

sDMD: An open source program for discontinuous molecular dynamics simulation of protein folding and aggregation

Size Zheng[a,*], Leili Javidpour[b], Muhammad Sahimi[c], Katherine S. Shing[c], Aiichiro Nakano[c]

*Quantum Science & Technology* **6**, 014007 (2021)

Domain-specific compilers for dynamic simulations of quantum materials on quantum computers

Lindsay Bassman[5,1], Sahil Gulania[2], Connor Powers[1], Rongpeng Li[3], Thomas Linker[1], Kuang Liu[1], T K Satish Kumar[4], Rajiv K Kalia[1], Aiichiro Nakano[1] and Priya Vashishta[1]

*Phys. Chem. Chem. Phys.* **24**, 10378 (2022)

**Probing the presence and absence of metal-fullerene electron transfer reactions in helium nanodroplets by deflection measurements†**

John W. Niman,[a] Benjamin S. Kamerin,[a] Thomas H. Villers,[a] Thomas M. Linker,[b] Aiichiro Nakano[b] and Vitaly V. Kresin*[a]

# More Class Projects (2)

Article https://doi.org/10.1038/s41467-024-47685-8

## Scalable computation of anisotropic vibrations for large macromolecular assemblies

Jordy Homing Lam[1,2,3], Aiichiro Nakano[1,4,5] & Vsevolod Katritch[1,2,3,6]

Nature Communications | (2024)15:3479

https://github.com/jhmlam/Inching

PHYSICAL REVIEW B **110**, 075116 (2024)

## Dynamics of symmetry-protected topological matter on a quantum computer

Miguel Mercado,[1,*] Kyle Chen,[2] Parth Hemant Darekar,[3,4] Aiichiro Nakano,[5] Rosa Di Felice,[1,6] and Stephan Haas[1]

JCIM JOURNAL OF CHEMICAL INFORMATION AND MODELING COMPUTATIONAL CHEMISTRY | September 11, 2024

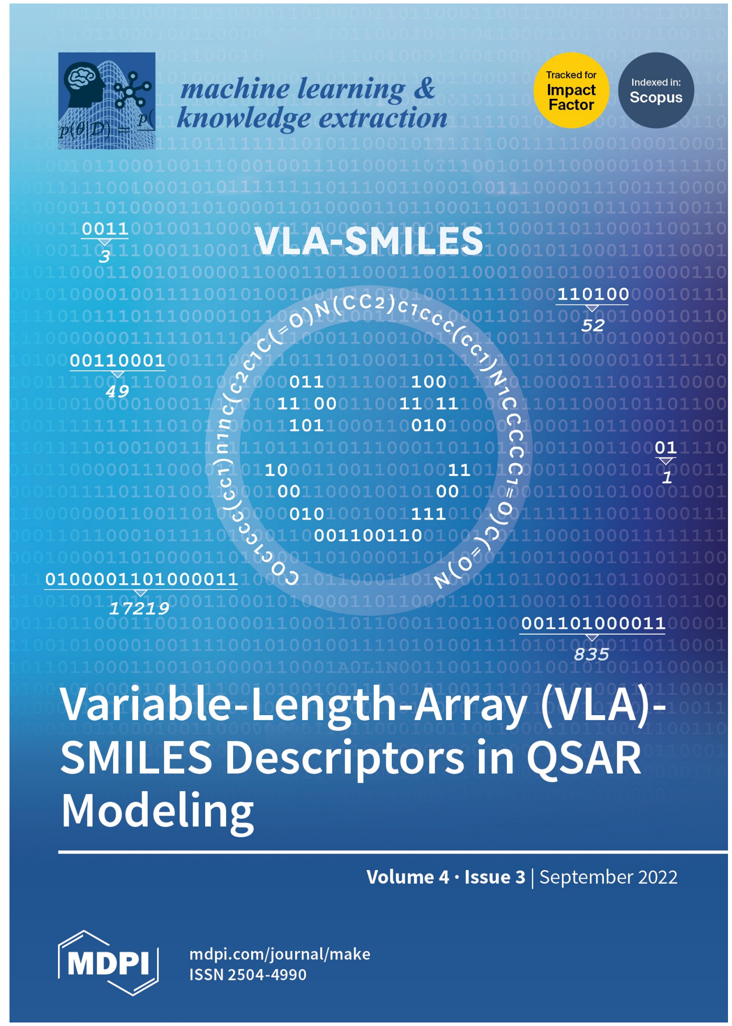
pubs.acs.org/jcim Article

## Exploring the Global Reaction Coordinate for Retinal Photoisomerization: A Graph Theory-Based Machine Learning Approach

Goran Giudetti,[⊥] Madhubani Mukherjee,[⊥] Samprita Nandi, Sraddha Agrawal, Oleg V. Prezhdo, and Aiichiro Nakano[*]

Cite This: https://doi.org/10.1021/acs.jcim.4c00325 Read Online

# More Class Projects: Journal Cover


Dielectric polymer property prediction using recurrent neural networks with optimizations

Antonina L. Nazarova, L. Yang, K. Liu, A. Mishra, R. K. Kalia, K. Nomura, A. Nakano, P. Vashishta, and P. Rajak

*Journal of Chemical Information and Modeling* **61**, 2175 ('21)

**VLA-SMILES: Variable-Length-Array SMILES Descriptors in Neural Network-Based QSAR Modeling**

**Antonina L. Nazarova [1,*,†] and Aiichiro Nakano [2,*]**

*Journal of Machine Learning and Knowledge Extraction* **4**, 715 (2022)

# Not Quite from This Class

nature computational science

Article

https://doi.org/10.1038/s43588-022-00370-6

## Fast multi-source nanophotonic simulations using augmented partial factorization

Received: 29 June 2022

Accepted: 10 November 2022

Published online: 15 December 2022

Check for updates

Ho-Chun Lin, Zeyu Wang & Chia Wei Hsu

Numerical solutions of Maxwell's equations are indispensable for nanophotonics and electromagnetics but are constrained when it comes to large systems, especially multi-channel ones such as disordered media, aperiodic metasurfaces and densely packed photonic circuits where the many inputs require many large-scale simulations. Conventionally, before extracting the quantities of interest, Maxwell's equations are first solved on every element of a discretization basis set that contains much more information than is typically needed. Furthermore, such simulations are often performed one input at a time, which can be slow and repetitive. Here we propose to bypass the full-basis solutions and directly compute the quantities of interest while also eliminating the repetition over inputs. We do so by augmenting the Maxwell operator with all the input source profiles and all the output projection profiles, followed by a single partial factorization that yields the entire generalized scattering matrix via the Schur complement, with no approximation beyond discretization. This method applies to any linear partial differential equation. Benchmarks show that this approach is 1,000–30,000,000 times faster than existing methods for two-dimensional systems with about 10,000,000 variables. As examples, we demonstrate simulations of entangled photon backscattering from disorder and high-numerical-aperture metalenses that are thousands of wavelengths wide.

Parallelized in CSCI 653

# Project in Another Class

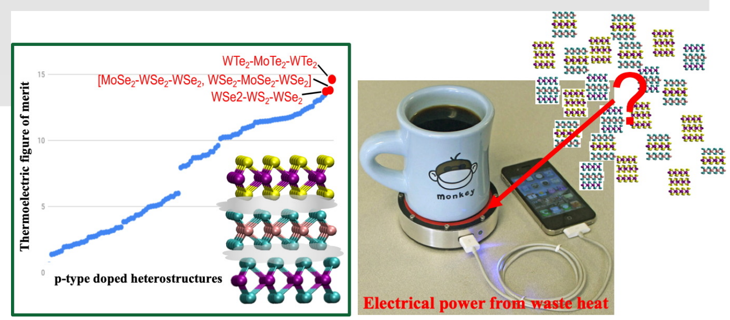
**ARTICLE** OPEN

## Active learning for accelerated design of layered materials

Lindsay Bassman[1,2], Pankaj Rajak[1,3], Rajiv K. Kalia[1,2,3,4], Aiichiro Nakano[1,2,3,4,5], Fei Sha[4,5], Jifeng Sun[6], David J. Singh[6], Muratahan Aykol[7], Patrick Huck[7], Kristin Persson[7] and Priya Vashishta[1,2,3,4]

Hetero-structures made from vertically stacked monolayers of transition metal dichalcogenides hold great potential for optoelectronic and thermoelectric devices. Discovery of the optimal layered material for specific applications necessitates the estimation of key material properties, such as electronic band structure and thermal transport coefficients. However, screening of material properties via brute force ab initio calculations of the entire material structure space exceeds the limits of current computing resources. Moreover, the functional dependence of material properties on the structures is often complicated, making simplistic statistical procedures for prediction difficult to employ without large amounts of data collection. Here, we present a Gaussian process regression model, which predicts material properties of an input hetero-structure, as well as an active learning model based on Bayesian optimization, which can efficiently discover the optimal hetero-structure using a minimal number of ab initio calculations. The electronic band gap, conduction/valence band dispersions, and thermoelectric performance are used as representative material properties for prediction and optimization. The Materials Project platform is used for electronic structure computation, while the BoltzTraP code is used to compute thermoelectric properties. Bayesian optimization is shown to significantly reduce the computational cost of discovering the optimal structure when compared with finding an optimal structure by building a regression model to predict material properties. The models can be used for predictions with respect to any material property and our software, including data preparation code based on the Python Materials Genomics (PyMatGen) library as well as python-based machine learning code, is available open source.

*npj Computational Materials* (2018)4:74 ; https://doi.org/10.1038/s41524-018-0129-0




***Involve your Ph.D. advisor in final discussion!***

**This is why our assignments were made intentionally easy; now apply the learned concepts/methods/tools to your "interesting problems"**


## Nonequilibrium Statistical Mechanics

Robert Zwanzig

## Table of Contents



asgn. 7-I & II

asgn. 7-III

# Preface

My intention in this book is to provide some understanding of the various methods that have been proposed for treating time-dependent processes in statistical mechanics. Some familiarity with equilibrium statistical mechanics is assumed. Whenever possible, I start with a simple example, generalize it, and finally discuss its theoretical foundations. The applications treated here were chosen as simple illustrations of a particular method; these choices were motivated by their utility in chemical physics. The methods, of course, have a much wider applicability, for example, in biophysics or condensed matter physics or even in astrophysics. There are no problem sets or exercises; most interesting problems are suitable subjects for serious research, and there is no point practicing on uninteresting problems. There are few literature references, only the occasional name and date; a lot of the material has been around a long time, and some of it is my own work.

In a letter accepting the Rumford medal of the American Academy of Arts and Sciences in 1881, J. Willard Gibbs wrote

> One of the principal objects of theoretical research in any department of knowledge is to find the point of view from which the subject appears in its greatest simplicity.

This is a hard standard; I hope that I came close. I am especially indebted to Attila Szabo, who encouraged me to finish a project I started about 1965 and who worked hard to get me to simplify my often obscure treatments of various topics. My failures are my own, not his.

# Final Brainstorming

- **Now, we all speak the common language to talk**
  - > **Assignment 1: Speak math/proof**
  - > **Vector space:** $1 = \sum_n |n\rangle\langle n|$
  - > **Dynamic system:** $\exp(\hat{H}t)$
  - > $\cdots$
- **Time to brainstorm crossing discipline boundaries**
  **~ minimum-energy pathways to innovation**
  - > **SVD, Krylov, Cholesky, …**
- **Let's have fun: please speak up!**