

On Final Projects

- **What? Anything You like**
- **Written report + presentation**
- **Either *Programming* or *Proposal***

Paper Abstract Format

The nature of free-carrier transport in organometal halide perovskites

Tomoya Hakamata¹, Kohei Shimamura^{1,2,3}, Fuyuki Shimojo¹, Rajiv K. Kalia², Aiichiro Nakano²
& Priya Vashishta²

Sci. Rep. **5**, 19599 ('16)

(1) Problem: Organometal halide perovskites are attracting great attention as promising material for solar cells because of their high power conversion efficiency. The high performance has been attributed to the existence of free charge carriers and their large diffusion lengths, but the nature of carrier transport remains unknown at the atomistic level. **(2) Finding:** Here, nonadiabatic quantum molecular dynamics simulations elucidate the mechanisms underlying the excellent free-carrier transport in $\text{CH}_3\text{NH}_3\text{PbI}_3$. Pb and I sublattices act as disjunct pathways for rapid and balanced transport of photoexcited electrons and holes, respectively, while minimizing efficiency-degrading charge recombination. On the other hand, CH_3NH_3 sublattice quickly screens out electrostatic electron-hole attraction to generate free carriers within 1 ps. Together this nano-architecture lets photoexcited electrons and holes dissociate instantaneously and travel far away to be harvested before dissipated as heat. **(3) So What?** This work provides much needed structure-property relationships and time-resolved information that potentially lead to rational design of efficient solar cells.

Paper Abstract Format (2)

Picosecond amorphization of SiO₂ stishovite under tension

Masaaki Misawa,^{1,2} Emina Ryu,² Kimiko Yoshida,³ Rajiv K. Kalia,¹ Aiichiro Nakano,^{1*} Norimasa Nishiyama,⁴ Fuyuki Shimojo,² Priya Vashishta,¹ Fumihiro Wakai³

Sci. Adv. 3, e1602339 ('17)



(1) Problem: 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. 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.

Punch-Kick Writing

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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 kicker. 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>

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?

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?

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".

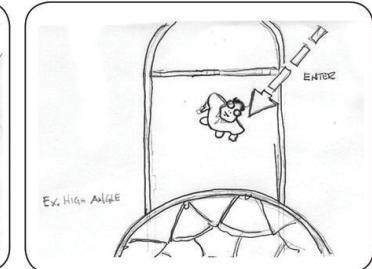
A paper is not just an archival device for storing a completed research program; it is also a structure for planning your research in progress. If you clearly understand the purpose and form of a paper, it can be immensely useful to you in *organizing* and conducting your research. A good outline for 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".

SHOT 23



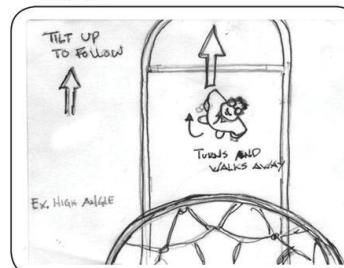
LONG SHOT: Billy walks out of door of office, throws hands into air and SOT shouts "YEAH" with glee! Maybe does a "Victory Dance" and pulls a lottery ticket out of his pocket.
SOT: ANNOUNCER VO: "The California State Lottery..."

SHOT 24



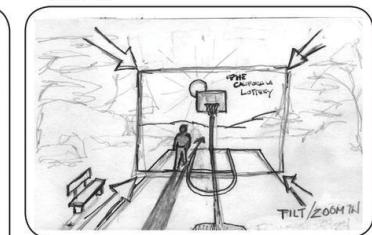
WIDE SHOT: Billy walks into the scene and tosses the wadded up report into the basketball net, While holding a Lottery Ticket in other hand.
SOT: ANNOUNCER: "...current jackpot now more than 25-million dollars..."

SHOT 25



CU: BILLY LOOKS UP through the basketball net then walks away.
GRFX: "California State Lottery.. Play to win."
ANNOUNCER VOICE OVER: "Play to Win!"

SHOT 26



LONG SHOT: Billy walks off into sunset. Hold long shot to cover VO.
ANNOUNCER VOICE OVER: [Extremely fast]
"The California State lottery is a legal gambling opportunity. The California State Lottery holds no responsibility for players with gambling addictions... " The California State Lottery recognizes those players have a better chance of being hit by lightning than winning the jackpot... "
"The California State Lottery holds no responsibility for loss of home or possessions of addicted players and acknowledges that investing that money in an IRA will give you a better chance of retirement than the Lottery. Please gamble responsibly." FADE TO BLACK
[FADE BILLY UP OVER VIDEO your choice of how to make credits]

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 Furukawa¹, Toshimori Sekine², Masahiro Oba³, Takeshi Kakegawa¹ & Hiromoto Nakazawa²

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 CSCI596 Team

International Journal of Computational Science

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2007, Vol. 1, No. 4, 407-421

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

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Aiichiro Nakano^{1*}, Priya Vashishta¹

material science
molecular dynamics
parallel

computer science
visualization
parallel

Another CSCI596 Team

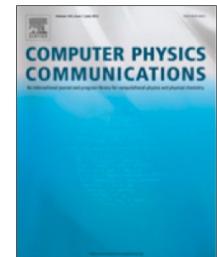
Computer Physics Communications 207 (2016) 186–192



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



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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

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JOURNAL OF APPLIED PHYSICS 111, 054907 (2012)

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

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O(N) Lanczos eigensolver (PHYS516) → parallelization (CSCI596)

Multi-Class Project (2)

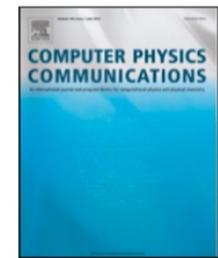
Computer Physics Communications 219 (2017) 246–254



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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

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CrossMark

Kinetic Monte Carlo (PHYS516) → parallelization (CSCI596)