On Final Projects

• What? Anything You like
• Written report + presentation
• Either Programming or Proposal
Picosecond amorphization of SiO$_2$ stishovite under tension

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(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!
Towards Dynamic Simulations of Materials on Quantum Computers

Lindsay Bassman et al.

(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

So what = kicker

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
Winning Pattern in Science

Why → So what → Now what

“Now what” by John Hopfield (Princeton)
https://pni.princeton.edu/john-hopfield/john-j.-hopfield-now-what
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)
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”.

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.

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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.