Ole Doc Lewis's Guide to Writing Scientific Papers

Steven Lewis

CSP Seminar

October 11, 2016

"How should I go about learning how to write a scientific paper?"

- I'll give you my perspective here.
- Talk to other professional scientists for their perspective (e.g., your advisor).
- Read papers in your field to get a sense of their style and structure.
  - What about them do you find most helpful?
  - What would you like to see done better?

"What should my mindset be as I write my paper?"

- A paper should tell a story. Decide what story you want to tell and how best to tell it.
- You're writing for your readers, so know your audience and *speak to them*.
- Realize that you know about your study in all it's gory detail, but your *readers do not*.
  - Always try to put yourself in the *mind of your reader* as you craft and edit your paper.
  - Don't assume your reader can read your mind!

"What should my mindset be as I write my paper?"

- Be aware of how people read papers:
  - First the title. If that draws reader's interest …
  - Then the abstract. If that keeps reader's interest …
  - Then the figures and tables. It often ends here, but if the reader wants more information …
  - Then the entire paper starting at the introduction.

Example: My First Doctoral Student's First Research Paper

Available online at www.sciencedirect.com
SCIENCE DIRECT®
Chemical Physics Letters 372 (2003) 836–841
CHEMICAL PHYSICS LETTERS
www.elsevier.com/locate/cplett

Weak bonding of carbon atoms at corner sites in titanium-carbide nanocrystals

Qin Zhang, Steven P. Lewis *

Department of Physics and Astronomy and Center for Simulational Physics, The University of Georgia, Athens, GA 30602-2451, USA

Received 3 February 2003; in final form 4 February 2003

Abstract

Recent experiments suggest that carbon atoms are disfavored at corner sites in transition-metal carbide nanocrystals. We examine this issue theoretically within density-functional theory, by focusing on the $3 \times 3 \times 3$ titanium-carbide nanocrystals: $Ti_{14}C_{13}$ and $Ti_{13}C_{14}$. The former species has metal atoms at the corners and is seen experimentally in great abundance, while the latter has carbon atoms at the corners and is not seen at all in the experiments. Our energetic and vibrational calculations indicate that carbon atoms are significantly more weakly bound to corner sites than are metal atoms. Possible consequences of these weakened corner-carbon bonds are discussed.

"Now that I'm in the right mind-set, where should I start?"

- Brainstorm a list of figures and tables that might help you tell the story.
  - Figures and tables form the "skeleton" on which the paper is built.
  - You may not end up using all of the figures and tables on your list.
  - Rough out what the figures and tables might look like; save final versions for later.

"Now that I'm in the right mind-set, where should I start?"

Example:

- FIGURES
  - Ball-and-stick figures of $Ti_{14}C_{13}$, $Ti_{13}C_{14}$, Ti_6C_{13}, $Ti_{13}C_6$
  - Displacement pattern for high-frequency A_{2u} mode for both $Ti_{14}C_{13}$ and $Ti_{13}C_{14}$
- TABLES
  - Relaxed structural parameters all four molecules
  - Average bond energy for all for molecules
  - Frequency of A_{2u} mode for $Ti_{14}C_{13}$ and $Ti_{13}C_{14}$

"Now that I'm in the right mind-set, where should I start?"

- Make a detailed outline of the paper before you ever start writing.
  - Allows you to organize your thoughts before having to worry about sentence structure, word choice, etc.
  - Gives you a "blue print" for the paper. You know what will go where; now you just have to put it into words.
  - Your outline need not be static. You can make changes or additions while you're writing.

"Now that I'm in the right mind-set, where should I start?"

I. Introduction
   A. Brief background on discovery of TMC nanocrystals and their potential applications.
   B. Brief description of structure of TMC nanocrystals and their relationship to bulk TMC crystals.
   C. Two noteworthy observations:
      1. $M_{14}C_{13}$ is VERY abundant, but $M_{13}C_{14}$ (also 3×3×3) is not seen *at all*.
         a. Other all-odd nanocrystals
         b. Small peak for $Ti_{13}C_6$ seen ➔ $Ti_{13}C_{14}$ minus its eight corner carbons
      2. For nanocrystals with at least one even dimension, no peak seen at the mass of the defect-free fragment. But peaks are seen at masses corresponding to n fewer carbon atoms, with n = 4 the largest.
   D. This paper presents our theoretical work examining this conclusion: Focus on $Ti_{14}C_{13}$ vs. $Ti_{13}C_{14}$

II. Systems and Methods
   A. Describe the systems we've studied to look at this issue
      1. Main: (a) $Ti_{14}C_{13}$, (b) $Ti_{13}C_{14}$, (c) Ti_6C_{13}, (d) $Ti_{13}C_6$
         a. Perhaps show models in a figure
         b. Comment on 3 (or 2) distinct bond types
      2. Secondary: (a) Isolate Ti atom, (b) Isolated C atom

"Now that I'm in the right mind-set, where should I start?"

2. Secondary: (a) Isolate Ti atom, (b) Isolated C atom

B. Describe the kinds of calculations we've done
   1. Computing relaxed structures and energies ➔ average Ti-C bond energies for each system (since only Ti-C bonds are present).
   2. Computing harmonic interatomic force constants ➔ bond strengths and normal modes and frequencies.

C. Briefly describe DFT method and relevant computational details (e.g., functional, pseudopotentials, plane waves, cutoffs, supercells, H-F forces, ...)

III. Results, Discussion, and Analysis

A. Relaxed structures ➔ More rounded corners for $Ti_{14}C_{13}$ than for $Ti_{13}C_{14}$

B. Average Ti-C bond energies ➔ Higher for $Ti_{13}C_6$ means bonds that were removed (those to corner carbons) were weaker

C. Bond-stretch force constants (and possibly others) ➔ Comparison of force constants for bonds to corner atoms

D. A_{2g} vibrational that red shifts *a lot* in going from $Ti_{14}C_{13}$ to $Ti_{13}C_{14}$ ➔ Analysis of mode pattern

E. Bring A.-D. all together ➔ bonds to corner carbons are weak!

F. Sketch out electronic explanation

IV. Conclusions (What goes here to be determined)

V. Acknowledgments (Mike Duncan, PRF grant, NSF grant, NCSA time)

"Any advice on the individual sections of the paper?"

- Introduction
  - This section is like a funnel, where you take the reader from the general area of interest to the specific question at hand.
  - It is often the hardest part to write. Until you get good at it, you may wish to start writing some other section first.
  - This section usually has the most references to other papers. (Methodology comes close.)

"Any advice on the individual sections of the paper?"

- Methodology
  - Unless the paper is about a new methodology, do not try to teach readers the methodology.
  - Give enough explanation so that a novice gets a sense of what the technique is/does, plus good references for interested readers to learn more.
  - Identify enough of the details so that an expert knows exactly what you did and can duplicate it if they wish.

"Any advice on the individual sections of the paper?"

- Conclusions
  - Summarize the main points of the paper and the conclusions that can be drawn.
  - Indicate any significant limitations on the scope of applicability of the work – terms left out, cases not considered, physics not included, etc.
  - Discuss important implications of the work, future avenues of investigation, etc.

"Any advice on the individual sections of the paper?"

- Title
  - I usually start with some working title and then spend time at the end crafting a good final title.
  - The title is important! It's the first thing a reader uses to decide whether or not to read further.
  - Good titles should not be excessively verbose, but should convey the main point of the paper.
  - Avoid using cute, clever titles until you're an established genius.

"Any advice on the individual sections of the paper?"

- Byline
  - With your first paper, choose how you want your name to appear on publications, and then stick with that for the rest of your career!
    - E.g., I use "Steven P. Lewis", not "S. P. Lewis" or "Steven Lewis" or …
  - Who is included as an author on the paper can be controversial (although usually not). Make sure you are aware of your discipline's ethical standards for authorship inclusion!

"Any advice on the individual sections of the paper?"

- Byline (cont'd)
  - Author ordering is a tricky issue, and different fields have different expectations. Here are my "rules of thumb":
    - The person who actually writes the paper goes first.
    - The group leader goes last.
    - Other authors go in between in order of significance of their contributions to the work.
    - The group leader generally has the final say.

"Any advice on the individual sections of the paper?"

- Abstract
  - I almost always wait until I've written the paper to write the abstract.
  - It should be a brief statement (~4-5 sentences) of what the paper is about and what the main results are.
  - A reader should get the gist of the paper from the abstract, even if they don't decide to read further.

"Any advice on the individual sections of the paper?"

- References
  - Best to use a reference manager application (e.g., EndNote, BibTeX).
  - It's tempting to save entering new references until the end, but trust me, that is the surest road to madness!
  - Be careful to follow the reference format for the journal you're submitting to.

"Any advice on the individual sections of the paper?"

- Figure and Table Captions
  - Some people prefer minimalist captions (e.g., "Susceptibility vs. Temperature").
  - I prefer captions with enough detail to make the figure or table as "self-contained" as reasonably possible.
  - For many "readers", all they'll look at are the title, abstract, figures, and tables. Useful captions make it easier on the reader.

"Any advice on the individual sections of the paper?"

- Acknowledgments
  - First off, this ↑ is the correct spelling in American English. (In British English, there is an extra 'e': Acknowledgements.)
  - Acknowledge grants whose support (financial, computer time, etc.) enabled the work.
  - Acknowledge people who made material contributions, but not enough for authorship.
  - Do not acknowledge family, friends, pets, etc.

"OK, I've written a draft of my paper. Now what?"

- Edit your work. Multiple times!
  - Most people don't edit as they go; they just get it down and worry about getting it right later.
  - Reading your draft aloud is very helpful. Your ear will catch things that your eye misses.
  - As you're editing, keep asking yourself, "Will my readers understand this, or do I need to clarify?"
  - Try to keep your prose tight, but clear. This is a skill that will only come with practice.

"OK, I've written a draft of my paper. Now what?"

- Proofread your work. Multiple times!
  - Proofreading means checking for correctness of spelling, usage, grammar, parallelism, etc.
  - Carefully check for mistakes in your figures and tables and their captions.
  - If English is not your native language, ask a friend who *is* a native English speaker to proofread it too for language-related issues.
    - A little "thank you" gift would be a nice touch.

"OK, I've written a draft of my paper. Now what?"

- Once all authors have signed off on the final draft, submit it to the journal!
  - Most journals explain on their website how to submit papers.
  - They also have information like style guides, etc.
- Finally, relax! For a few minutes only, and then get back to work! ☺