Constructing and writing a scientific paper

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PH 4/591 Fall 2022

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This is a “W” class

- As such, we require 2 papers
- One with feedback around midterm
- One at the end
- In both cases, you will be able to revise & resubmit if you like, based on my feedback
- First one due 29 Sept – basic design of your experiment and progress report

What we'll do (and won't)

- We will discuss:
  - What is particular to writing a scientific paper
  - What are some good and bad practices
  - Look at and critique specific examples
- We will not discuss
  - Language, grammar, etc.
  - Details about specific programs

To write you need to read

- “Scientific English” is not well-defined
  - but people know it when they see it
- Read papers in your area, get a feel for style
- But *don’t* take what you see as gospel – pay attention to what you don’t like too
- Also - necessary to contextualize your work
- Will use my own examples, good and bad

Basic content guidelines

- Well-organized, clear argument start → finish
- Know your audience …
- Know the destination requirements
  - e.g., https://journals.aps.org/prl/authors
- Don’t make up new terms unless you must
- Set off equations rather than inline
- Put work in context, make clear what is new/different

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Basic format of a journal article

- Obviously varies. Example for expt + theory
- Title, abstract
- Introduction – background, what has been done, what did you do
- Methods
- Results & Discussion
- Conclusions
- Acknowledgements
- References

First a short tour of each section
Then do’s and don’t’s
Then how to go about it

Title and abstract

- Title: catchy but true.
  - Concise and informative. Avoid hyperbole
  - If your title doesn’t catch someone’s eye, they will never read the rest.
  - Must give an idea of what the paper is about
- Abstract:
  - the second, and possibly last thing anyone reads
  - Succinct, self-contained.
  - Summarize the whole work, key points
- I usually finish title last, abstract second to last!

$Co_2Fe_{1.25}Ge_{0.75}$: A single-phase full Heusler alloy with highest magnetic moment and Curie temperature

Material and what we found clear
(maybe not 'catchy' ...)

Check for updates

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A R T I C L E I N F O

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Keywords:
Transition metal alloys and compounds
Solid state reactions
Crystal structure
Magnetism
X-ray diffraction
Thin films
Density functional theory

Summarize key points of whole work

First and last sentences key.

A B S T R A C T

Elemental substitution by a different element is a well utilized technique of stabilizing a single-phase compound, in case the parent alloy is multi-phase, and this has been demonstrated specifically in a number of Heusler systems. This can, however, give an increased propensity for chemical disorder as well as adding complexity to synthesis and characterization.

In this paper, we present the successful synthesis of a single-phase compound, $Co_2Fe_{1.25}Ge_{0.75}$, by tuning the parent Co_2FeGe stoichiometry (which exhibits multi-phase structure) rather than introducing a fourth element. The compound is found to crystallize in $L2_1$ structure (space group # 225). Magnetization measurements reveal $Co_2Fe_{1.25}Ge_{0.75}$ has a saturation magnetization as high as 6.7 ± 0.1 μ_B/f.u. at 5 K and a Curie temperature of 1135 ± 5 K – both being the highest reported to date for cubic full Heusler alloys to our knowledge. Thin films of $Co_2Fe_{1.25}Ge_{0.75}$ deposited on $Al_2O_3(110)$ and $MgAl_2O_4(100)$ substrates show excellent expitaxial quality, among the reported for Heusler films to date, and exhibit magnetic properties comparable to bulk samples. First principle calculations suggest the system exhibits total energy minimum at the experimentally-observed lattice parameter. Furthermore, the calculations corroborate the observed enhancement in magnetization and point to the importance of on-site Coulomb interactions. While our novel approach of substitution led to the discovery of stable $Co_2Fe_{1.25}Ge_{0.75}$ alloy with very high moment and Curie temperature that can be readily grown as a high-quality epitaxial thin film, making it a candidate for device applications, this approach can be taken as a new paradigm for the discovery of novel single-phase Heusler compounds with enhanced magnetic properties.

Introduction

- Probably third to last … because it informs the rest of the paper (and therefore relies on it existing)
- What is the basic motivation?
- What has been done before?
- What issues remain?
- What did you do?
- https://doi.org/10.1016/j.jallcom.2018.07.298

Methods

- This part is simple enough.
- List the stuff you used and how you used it
- But add the *details* – enough to reproduce
  - Which tool did you use?
  - Which algorithm?
  - What conditions?
- Most journals now have “supplementary info” docs you can add so length is no worry

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Example

II. METHODS

A. Experimental methods

The bulk $Co_{2-x}Cr_xFeGe$ $(0 \leqslant x \leqslant 1)$ stoichiometric Heusler alloys were prepared by melting Co, Fe, Cr, and Ge pieces of 99.99% purity in an arc furnace on a Cu hearth provided with water cooling under argon flow at a base pressure of 10^{-4} mbar. The mixture was melted at least 6 times to ensure chemical homogeneity. As an oxygen getter, Ti was melted inside the vacuum chamber separately before melting the compound to avoid oxygen contamination. The weight loss during the process was negligible. The resulting ingots were cut into pieces and examined using an energy dispersive x-ray spectroscopy (EDS) detector equipped in a JEOL 7000 field emission scanning electron microscope (FESEM) to ensure the target composition after the arc melting. These pieces were annealed in evacuated quartz tubes for different heat treatments, and cooled slowly in the furnace to get optimum crystallization to promote the formation of $L2_1$ structure. To make the comparison uniform across all compositions, only the samples annealed under similar heat treatments (i.e., 1000 °C for 15 days) are reported. The heat treatments were followed by metallography (see details in the Supplemental Material [46]) to produce a metallic shiny surface for microstructure analysis by optical and electron microscopes. After the heat treatment and metallography, the composition and homogeneity of the samples were again confirmed by using EDS.

Structural analysis was carried out by using x-ray diffraction (XRD) using a Bruker D8 Discover x-ray diffractometer equipped with monochromatic Co-Kα ($\lambda = 0.179$ nm) radiation. The polished samples were rotated around the ϕ axis during the XRD measurement to minimize surface effects. CARINE crystallography 4.0 software [47] as well as in-house PYTHON code [48] including the dispersive corrections to the atomic scattering factors were used to simulate the XRD patterns to compare with the experimental XRD patterns. Rietveld refinement was done using a MATCH! software based on the FULLPROF algorithm [49]. The low-temperature magnetic properties were studied in Quantum Design Physical Properties Measurement System (PPMS), while the high-temperature magnetization was measured using LakeShore VSM 7407. The mechanical properties were studied in terms of Vickers hardness by using Buehler model 1600-6100 micro-hardness tester.

B. Computational methods

We have performed density functional theory (DFT) calculations employing the projector augmented wave (PAW) pseudopotentials by Blöchl [50], implemented by Kresse and Furthmüller in the Vienna *ab initio* simulation package (VASP) [51]. We have adopted the generalized gradient approximation (GGA) in the scheme of Perdew, Burke, and Ernzerhof (PBE) for the electronic exchange-correlation functional [52]. We have used a 16-atom supercell, i.e., 4 formula units of the underlying $L2_1$ structure adopted by the perfect full-Heusler compounds like Co_2MnGe. The integration over the irreducible Brillouin zone (IBZ) of cubic systems was done with the automatic mesh generation scheme within VASP with the mesh parameter (the number of k points per Å^{-1} along each reciprocal lattice vector) set to 30, which generates a $10 \times 10 \times 10$ Γ-centered Monkhorst-Pack grid in the case of cubic lattices [53]. Total energies were converged upto 10^{-7}eV/cell with a plane-wave cutoff of 520 eV. Full re-

Results and discussion

- This is what it sounds like
- Break into sub-sections if necessary
- Proceed logically rather than historically
- *Include negative results that are relevant*
- First describe, then analyze
- OK to speculate, but be clear when you are
- https://doi.org/10.1103/PhysRevMaterials.3.114406

Conclusions/acknowledgements

- Like the abstract, but with the benefit of having read the paper
- What were the most important things?
- Entirely possible someone reads
  - Title → abstract → figures → conclusion
- Acknowledgements:
  - Funding, facilities used, helpful discussions, etc.

References

- Follow the style of the journal/publication
- Enough detail to actually find it
- *Actually read the papers you cite* at least briefly
- *Cite useful papers*
  - Often obliged to cite first paper, but also add the ones you found useful
  - Look at references and citations of papers you cite. Did you miss anything?

How do I write a paper

- Figure out the story first – rough outline
- Tell the story in pictures (figures)!
  - Visual outline of your work
- Describe each picture – the results section
- Discuss what they meant – discussion section
- Describe how you did each thing – methods
- This is already the bulk of your paper

How do I write a paper

- Can you summarize the whole thing succinctly?
  - This is your conclusion
- Can you explain why you did it and put it in context?
  - This is your introduction
- Can you write a 300-word sales pitch that summarizes everything? The *Abstract*.

How do I write a paper

- Throughout: what can I cite to justify what I just wrote? References.
- *Especially* in the introduction
- Now you need a catchy title

This presupposes you settled questions of formatting and style before starting.

Figures

- We talked about visualization
- Consistency and attention to detail
  - Same axis format, font sizes, units, etc.
- *Careful* with color – reading B&W printout? R/G colorblind? Use color strategically
- They can get too busy very easily

Tables

- Going back to visualization …
- Never use vertical rules (or grid)
- Forget double rules too
- Put units in the column heading, not table body
    - Redundant repetition and waste of valuable space

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Publication quality tables in LATEX, Simon Fear

LaTeX examples

- Hodge-podge of information.

gnats	gram	$13.65
	each	.01
gnu	stuffed	92.50
emu		33.33
armadillo	frozen	8.99

Publication quality tables in LATEX, Simon Fear

LaTeX examples

- Better, and easier to lay out

Item		
Animal	Description	Price ($)
Gnat	per gram	13.65
	each	0.01
Gnu	stuffed	92.50
Emu	stuffed	33.33
Armadillo	frozen	8.99

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Publication quality tables in LATEX, Simon Fear

Your schedule

- Very light grey to denote weeks and guide the eye – easy to get lost reading across
- Still too much text tbh

Date	Topic	Assignment given	Assignment due
18 Aug	Course intro, meet & greet.	inverse Occam's razor; finding info	
23 Aug	Case studies in experiment design	Paper critique/case study	
25 Aug	mini-experiments 1		Occam response + finding information
30 Aug	analysis & visualization of data	data visualization exercises	Paper critique
1 Sep	mini-experiments 2; discuss longer expts.		
6 Sep	writing a paper; pick longer expts.	paper outline for mini expt.	visualization exercises
8 Sep	first day with longer expts.		
13 Sep	curve fitting & analysis; longer expts.	curve fitting task	paper outline
15 Sep	continue with longer experiments		deliverable: preliminary data
20 Sep	electrical measurements & noise		curve fitting
22 Sep	continue with longer experiments		deliverable: initial analysis, supplies needed
27 Sep	feedback & control	(finish 1st round of expt. refinements	
29 Sep	continue with longer experiments		first paper due (expt. design & progress)
4 Oct	apparatus deep dive, discuss 1st paper	first paper feedback	
6 Oct	switch/continue longer experiments		deliverable: plan of work
11 Oct	discussion - status reports		
13 Oct	continue with experiments		
18 Oct	continue with experiments		deliverable: plan of work update
20 Oct	continue with experiments		first paper revisions due
25 Oct	continue with experiments		
27 Oct	continue with experiments		deliverable: data update/comparison
1 Nov	continue with experiments		
3 Nov	continue with experiments		final paper *outline* due
8 Nov	continue with experiments		
10 Nov	continue with experiments	feedback on final paper outline	
15 Nov	analysis & writing		
17 Nov	analysis & writing		final paper due
29 Nov	final presentations (grads)		
1 Dec	post mortem		

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Bad example

- Prominent top position has least important information

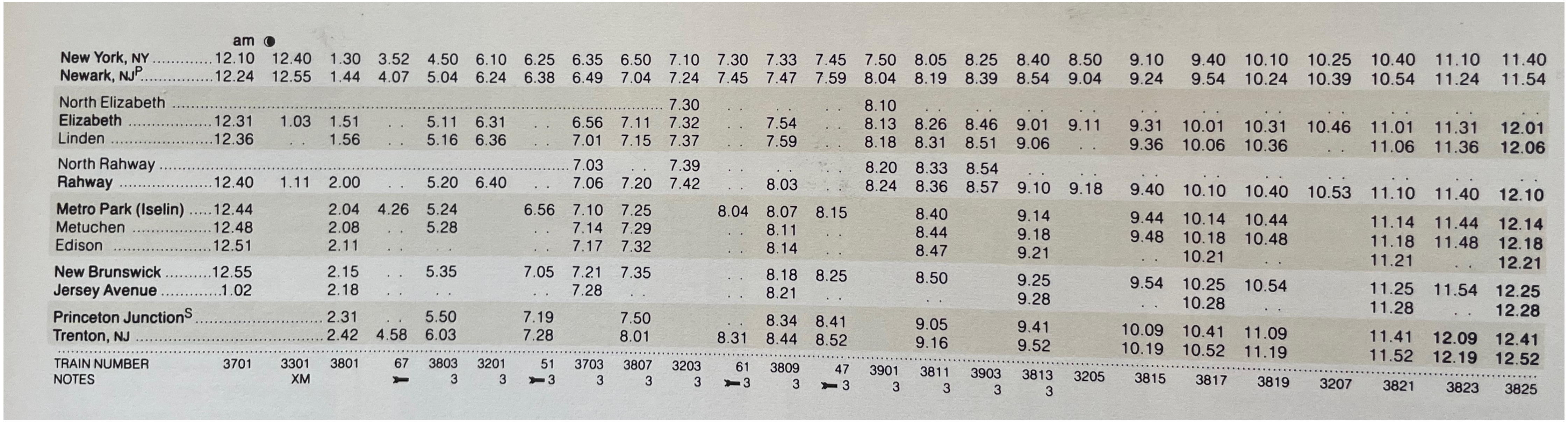
Train No.	3701	XM 3301	3801	A 67	3 3803	3 3201	A3 51	.3 3703	3 3807	3 3203	A3 61	3 3809	A3 47
	A.M.	A.M.	A.M.	A.M.	A.M.	A.M.	A.M.	A.M.	A.M.	A.M.	A.M.	A.M.	A.M.
New York, N.Y.	12.10	12.40	1.30	3.52	4.50	6.10	6.25	6.35	6.50	7.10	7.30	7.33	7.45
Newark, N.J. P	12.24	12.55	1.44	4.07	5.04	6.24	6.38	6.49	7.04	7.24	7.45	7.47	7.59
North Elizabeth	....	....	....	....	....	....	....	....	....	7.30	....	....	....
Elizabeth	12.31	1.03	1.51	....	5.11	6.31	....	6.56	7.11	7.32	....	7.54	....
Linden	12.36	....	1.56	....	5.16	6.36	....	7.01	7.15	7.37	....	7.59	....
North Rahway	....	....	....	....	....	....	....	7.03	....	7.39	....	....	....
Rahway	12.40	1.11	2.00	....	5.20	6.40	....	7.06	7.20	7.42	....	8.03	....
Metro Park (Iselin)	12.44	....	2.04	4.26	5.24	....	6.56	7.10	7.25	....	8.04	8.07	8.15
Metuchen	12.48	....	2.08	....	5.28	....	....	7.14	7.29	....	....	8.11	....
Edison	12.51	....	2.11	....	....	....	....	7.17	7.32	....	....	8.14	....
New Brunswick	12.55	....	2.15	....	5.35	....	7.05	7.21	7.35	....	....	8.18	8.25
Jersey Avenue	1.02	....	2.18	....	....	....	....	7.28	....	....	....	8.21	....
Princeton Jct. S	....	....	2.31	....	5.50	....	7.19	....	7.50	....	....	8.34	8.41
Trenton, N.J.	....	....	2.42	4.58	6.03	....	7.28	....	8.01	....	8.31	8.44	8.52

Train No.	3 3901	3 3811	3 3903	3 3813	3205	3815	3817	3819	3207	3821	3823	3825	.3209	3827	3829	3831
	A.M.	A.M.	A.M.	A.M.	A.M.	A.M.	A.M.	A.M.	A.M.	A.M.	A.M.	A.M.	A.M.	P.M.	P.M.	P.M.
New York, N.Y.	7.50	8.05	8.25	8.40	8.50	9.10	9.40	10.10	10.25	10.40	11.10	11.40	11.50	12.10	12.40	1.10
Newark, N.J. P	8.04	8.19	8.39	8.54	9.04	9.24	9.54	10.24	10.39	10.54	11.24	11.54	12.04	12.24	12.54	1.24
North Elizabeth	8.10	....	....	....	....	....	....	....	....	....	....	....	....	....	....	....
Elizabeth	8.13	8.26	8.46	9.01	9.11	9.31	10.01	10.31	10.46	11.01	11.31	12.01	12.11	12.31	1.01	1.31
Linden	8.18	8.31	8.51	9.06	....	9.36	10.06	10.36	....	11.06	11.36	12.06	....	12.36	1.06	1.36
North Rahway	8.20	8.33	8.54	....	....	....	....	....	....	....	....	....	....	....	....	....
Rahway	8.24	8.36	8.57	9.10	9.18	9.40	10.10	10.40	10.53	11.10	11.40	12.10	12.18	12.40	1.10	1.40
Metro Park (Iselin)	....	8.40	....	9.14	....	9.44	10.14	10.44	....	11.14	11.44	12.14	....	12.44	1.14	1.44
Metuchen	....	8.44	....	9.18	....	9.48	10.18	10.48	....	11.18	11.48	12.18	....	12.48	1.18	1.48
Edison	....	8.47	....	9.21	....	....	10.21	....	....	11.21	....	12.21	....	....	1.21	....
New Brunswick	....	8.50	....	9.25	....	9.54	10.25	10.54	....	11.25	11.54	12.25	....	12.54	1.25	1.54
Jersey Avenue	....	....	....	9.28	....	....	10.28	....	....	11.28	....	12.28	....	....	1.28	....
Princeton Jct. S	....	9.05	....	9.41	....	10.09	10.41	11.09	....	11.41	12.09	12.41	....	1.09	1.41	2.09
Trenton, N.J.	....	9.16	....	9.52	....	10.19	10.52	11.19	....	11.52	12.19	12.52	....	1.22	1.52	2.20

Tufte, “Envisioning Information”

Fixed

- Calmer without grid, most important at top
- De-emphasize less important data
- Adds new info, leader dots & shading gently guide



	am ◑																								
New York, NY	12.10	12.40	1.30	3.52	4.50	6.10	6.25	6.35	6.50	7.10	7.30	7.33	7.45	7.50	8.05	8.25	8.40	8.50	9.10	9.40	10.10	10.25	10.40	11.10	11.40
Newark, NJ[P]	12.24	12.55	1.44	4.07	5.04	6.24	6.38	6.49	7.04	7.24	7.45	7.47	7.59	8.04	8.19	8.39	8.54	9.04	9.24	9.54	10.24	10.39	10.54	11.24	11.54
North Elizabeth										7.30	. .	. .	. .	8.10	. .	. .	. .	. .	. .	. .	. .	. .	. .	. .	. .
Elizabeth	12.31	1.03	1.51	. .	5.11	6.31	. .	6.56	7.11	7.32	. .	7.54	. .	8.13	8.26	8.46	9.01	9.11	9.31	10.01	10.31	10.46	11.01	11.31	12.01
Linden	12.36	. .	1.56	. .	5.16	6.36	. .	7.01	7.15	7.37	. .	7.59	. .	8.18	8.31	8.51	9.06	. .	9.36	10.06	10.36	. .	11.06	11.36	12.06
North Rahway								7.03	. .	7.39	. .	. .	. .	8.20	8.33	8.54	. .	. .	. .	. .	. .	. .	. .	. .	. .
Rahway	12.40	1.11	2.00	. .	5.20	6.40	. .	7.06	7.20	7.42	. .	8.03	. .	8.24	8.36	8.57	9.10	9.18	9.40	10.10	10.40	10.53	11.10	11.40	12.10
Metro Park (Iselin)	12.44		2.04	4.26	5.24		6.56	7.10	7.25		8.04	8.07	8.15		8.40		9.14		9.44	10.14	10.44		11.14	11.44	12.14
Metuchen	12.48		2.08	. .	5.28		. .	7.14	7.29		. .	8.11	. .		8.44		9.18		9.48	10.18	10.48		11.18	11.48	12.18
Edison	12.51		2.11	. .	. .		. .	7.17	7.32		. .	8.14	. .		8.47		9.21		. .	10.21	. .		11.21	. .	12.21
New Brunswick	12.55		2.15	. .	5.35		7.05	7.21	7.35		. .	8.18	8.25		8.50		9.25		9.54	10.25	10.54		11.25	11.54	12.25
Jersey Avenue	1.02		2.18	. .	. .		. .	7.28	. .		. .	8.21	. .		. .		9.28		. .	10.28	. .		11.28	. .	12.28
Princeton Junction[S]			2.31	. .	5.50		7.19		7.50		. .	8.34	8.41		9.05		9.41		10.09	10.41	11.09		11.41	12.09	12.41
Trenton, NJ			2.42	4.58	6.03		7.28		8.01		8.31	8.44	8.52		9.16		9.52		10.19	10.52	11.19		11.52	12.19	12.52
TRAIN NUMBER	3701	3301	3801	67	3803	3201	51	3703	3807	3203	61	3809	47	3901	3811	3903	3813	3205	3815	3817	3819	3207	3821	3823	3825
NOTES		XM		➤	3	3	➤ 3	3	3	3	➤ 3	3	➤ 3	3	3	3	3								

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Tufte, “Envisioning Information”

Some things not to do

- It isn’t a story, exactly. “and then, and then …”
- It doesn’t have to be boring though!
- Be honest even though it is hard to write about what didn’t work or what you don’t understand
- Don’t feel pressured to mimic the style you read in every detail!
- Don’t dance around what you recognized but didn’t understand!

Some things not to do

- There are a *lot* of boring or pretentious-sounding papers.
- Tedium and opacity do not make it scientific
  - Using $5 words for $1 ideas – that first article we read
- Avoid exclusionary jargon and acronyms
  - We don’t print stuff anymore; do you really need to save characters?
  - Clearly define each acronym on first use
  - E.g., Co_2FeO_4 and Co_2MnSi --> CFO and CMS.
    - *Why? What would Co_2MnSn be then?*

Some things to do

- Read target journal to see if they have a particular style
- Make a good outline so your argument is crisp
- *Get someone else to read it*
- *Proofread, proofread, proofread*
- Look at every section and sentence, is there anything you don't need?

Some things to do

- Are you writing the same introduction everyone else does? If so, maybe don’t.
- It is *easy* to shorten a good draft, it is hard to add length meaningfully – write a good draft and worry about length later
- Make up your story and outline before you decide the destination – don’t add artificial constraints (e.g., page limit)

A few examples to look over

- Recent one, liked the intro:
  - https://www.sciencedirect.com/science/article/pii/S1359645422004931?via%3Dihub
- An older one, tried to cram too much into a page limit and it shows
  - https://journals.aps.org/prl/abstract/10.1103/PhysRevLett.94.037006
- Concise, decent figures; rare case of color contour/scale I didn't hate
  - http://dx.doi.org/10.1063/1.3654121
- A 1.5-pager that got a Nobel
  - https://journals.aps.org/prl/abstract/10.1103/PhysRevLett.5.147

Collaborative editing

- Overleaf (LaTeX)
- Box notes
- Box + office
- *Don't* email drafts back and forth like its 1998
- Set standards before you start
  - E.g., fonts, figure details, citations …
- *Communicate* – who's going to do what?

A good approach to group editing

- https://hbr.org/2021/07/a-better-approach-to-group-editing
- Limit participation
- Give enough time, but specific deadline
- Clarify roles – manager/writer/reviewer/approver
- Start with a clean draft – one expert, one writer
- Keep people in their lanes (writer vs subject expert)
- Share clean versions, maintain version control
- Explain *why* changes were made
- Indicate intention with each version

What about talks?

- A whole new ballgame
- Visualization stuff is crucial
- Some aspects translate, but now *performance* is also key
- A good start from our associate dean:
  - http://pages.astronomy.ua.edu/white/webtalks/raysrules.html

Paper pseudocode/outline

- For one of the mini-experiments
- I'll provide some data/figures/analysis
  - Focus on writing not visualization here
- Make detailed outline of the paper you would write
- Like pseudocode – outline + sketch of specific paragraphs

Rest of class

- Discuss longer experiments
- Pick groups (mostly done I guess)
- Pick your experiment to start with

- Next time we get started on them!
  - I’ll have some reading for you