PHY 7097: Molecular Magnetims **Fall 2019** **Professor Mark W. Meisel**

"*in vivo*" schedule (**black text: projected and tentative**; **purple text: past**; **blue text: hotlinks**; **red text important announcements**; **green text: fixed final exam**)

Note: Schedule is "projection" and revisions will be announced in class and subsequently posted online.

Week 1	Aug 20	Class Starts, Introduction to the Course
Lecture 1		**Molecular Magnetism Web** thanks to Jürgen Schnack
		Molecule-based Magnets – An Overview, J.S. Miller and A.J. Epstein, *MRS Bulletin* 25 (2000) 21-30 http://dx.doi.org/10.1557/mrs2000.221
		Jargon and Perspective: Green Tree Snake
		Family Tree of Magnetism, C.M. Hurd, *Contemp. Phys.* 23 (1982) 469-493.
	Aug 22	Discuss HW of setting schedule for meeting times of course.
Lecture 2		Answers to "self-test" and "homework" about LRO (long-range-order).
		The issue of length scales: one example of what Meisel is pondering
		Blather-meter installed…
		http://iopscience.iop.org/1367-2630/9/7/222/
		"one road to discovery"
Week 2	Aug 27	Magnetism – the start, the basics, things to know, things I wish I knew.
Lecture 3		E-Learning for PHY7097 posted, and now PUBLISHED!
		C.P. Landee, M.M. Turnbull, "Review: A gentle introduction to magnetism: units, fields, theory, and experiment", J. Coord. Chem. 67 (2014) 375-439.
		Finish story of "one road to discovery" see Lecture 2.
	Aug 29	Magnetism – the basic places to find information.
Data-Analysis-1		Let's get some data and start the analysis!
Week 3	Sep 03	Hurricane Day, UF closed. No class.
	Sep 05	Interactive Day in Small Group Projects, with guidance from the instructor.
		Modern reference about Spin Crossover (SCO) phenomena:

"A critical review of the T(LIESST) temperature in spin crossover materials – What it is and what it is not", G. Chastanet, C. Desplanches, C. Baldé, P. Rosa, M. Marchivie, P. Guionneau, *Chem Sq*., 2 (2018) 2, https://doi.org/10.28954/2018.csq.07.001

Reading for Next Week:

"Modification of Molecular Spin Crossover in Ultrathin Films", A. Pronschinske, Y. Chen, G.F. Lewis, D.A. Shultz, A. Calzolari, M. Buongiorno Nardelli, D.B. Dougherty, *Nano Lett*. 13 (2013) 1429-1434, https://doi.org/10.1021/nl304304e

"Molecular-scale dynamics of light-induced spin cross-over in a two-dimensional layer", K. Bairagi, O. Iasco, A. Bellec, A. Kartsev, D. Li, J. Lagoute, C. Chacon, Y. Girard, S. Rousset, F. Miserque, Y.J. Dappe, A. Smogunov, C. Barreteau, M.-L. Boillot, T. Mallah, V. Repain, *Nature Communications* 7 (2016) 12212, doi:10.1038/ncomms12212

Week 4	Sep 10		Finish Data-Analysis-1 discussion. Post report with text and data. Discussion of A. Pronschinske *et al*., *Nano Lett*. 13 (2013) 1429 paper. **Discussion of Primary, Secondary, Tertiary topics that you want covered.**
	Sep 12		Discussion of K. Bairagi *et al*., *Nature Commun*. 7 (2016) 12212 paper.
Week 5	Sep 17		Detailed discussion of SCO and LIESST.
	Sep 19		What can be measured and what can it tell you?
		(1)	Corrections for diamagnetic "supporting stuff"? Pascal's Constants: see "Diamagnetic Corrections and Pascal's Constants", G.A. Bain and J.F. Berry, *J. Chem. Educ.*, 2008, 85 (4), 532-536, DOI: 10.1021/ed085p532
		(2)	$\chi \times T$ at Room Temperature not "spin only" value? Then spin-orbit interactions persist to 300 K? Try, for example: "Magnetic functions beyond the spin-Hamiltonian", volume editor: D.M.P. Mingos ; with a contribution by R. Boča. Published: Berlin ; New York : Springer, 2006. UF Library E-book Full citation: Bocă , R. In *Magnetic Functions Beyond the Spin-Hamiltonian*; Mingos, D. M. P., Ed.; Springer-Verlag: Berlin, 2006; Vol. 117, pp 1− 264.
		(3)	**EasySpin** in MatLab environment.
Week 6	Sep 24		**Individual (15 min) meetings with Instructor.** (a) How is the course going? (b) What topics do you want to discuss? (c) Ideas/questions related to your project and one-pager?
	Sep 26		**Reading/Modelling Day:** An introduction to magnetism in three parts by Wulf Wulfhekel ***Cartoon*** of Fe(II) SCO active in microscopic terms?
			K.J. Anderton, D.M. Ermert, P.A. Quintero, M.W. Turvey, M.S. Fataftah, K.A. Abboud, M.W. Meisel, E. Čižmár, L.J. Murray, "Correlating Bridging Ligand with Properties of Ligand-Templated $[MnII_3X_3]^{3+}$ Clusters (X = Br^-, Cl^-, H^-, MeO^-), *Inorg. Chem*. 56 (2017) 12012-12022, doi:10.1021/acs.inorgchem.7b02004 ***Check*** model parameters using **EasySpin**?
Week 7	Oct 01		**Reading/Modelling Day:** A.E. Thuijs, X.-G. Li, Y.-P. Wang, K.A. Abboud, X.-G. Zhang, H.-P. Cheng, G. Christou, "Molecular analogue of the perovskite repeating unit and evidence for direct MnIII-CeIV-MnIII exchange coupling pathway", *Nature Commun*. 8 (2017) 500, doi: 10.1038/s41467-017-00642-0 **List** up to 3 "take-home" points and/or "curious" issues?
	Oct 03		**Reading/Modelling Day:** **Outline of your proposed project (one-pager).**

Week 8	Oct 08	Review past two weeks. Start Jahn-Teller Effect and Ligand Field Theory.
	Oct 10	**Meet with Instructor as needed to complete your project one-pager**. (0830 hrs to Noon, appointment by email, may be in NPB B133)
Week 09	Oct 15	Recap where we are and where we are going. Two topics to "finish". (1) Jahn-Teller Effect and Ligand Field Theory and the possibility of "issues" with Thuijs et al. paper, see Oct 01 entry. **Course requirements:**

One "project", pre-approved by instructor, and classroom presentation (20 min). "Intellectual Merit" (40%)
One outreach "spot" (the elevator speech) or "K-8 activity". "Broader Impacts" (40%)
A one-pager about where you started and where you finished the wild ride. (20%)

		HW (due by 23:59 hrs on Oct 15!): email me one-pager about "Project" and include statement about outreach "spot". **Meisel to discuss possibilities of joining expeditions to schools.**
	Oct 17	Michael Turner (University of Chicago) Colloquium at 4 pm in NPB 1002 "How many numbers does it take to determine our Universe?" Very similar to YouTube video of talk at Brown University, 11 March 2019 Reception in NPB 2205 to recognize Sakuari Prize 2019 receipent Pierre Sikivie. "Outreach/Broader Impacts Day."
Week 10	Oct 22	Two topics to "finish". (2) NMR and EPR: essentials and Other Experimental techniques. If time, Antiferromagnetic Spin Modes in $CuSe_2O_5$.

"Spin Dynamics in an Antiferromagnet", Marc Philipp Ross, Diploma thesis (2013) TU-München (PDF).

AND a Topic to Start by working in mini-groups:
SMM discussion begins (with goal of understanding the role of substrates).
Introduction to Molecular Magnetism (Joris van Slageren, Universität Stuttgart)
Elementary Magnetic Excitations in AntiferromagneticMolecular Nanomagnets (Dr. Waldmann, University of Bern)

	Oct 24	Discussion about "projects". SMM discussion, AC magnetic response, and surfaces.
Week 11	Oct 29	SMM discussion will continue, What is the buzz about Fe8.
	Oct 31	Professor Anupam Garg, Department of Physics and Astronomy, Northwestern University, Department of Physics Colloquium: "Magnets that find it hard to relax" 4 pm, NPB 1002, please attend if you schedule permits.

Abstract:
Many processes in nature, such as alpha decay of U-238, or the conversion of ortho to para hydrogen, take place very slowly, and in each case, an investigation into the causes teaches us important physics. In this talk, we will discuss magnetic relaxation in single molecule magnets such as Fe8, which is also very slow, but for completely different reasons than the previous two examples.

At low temperatures, Fe8 displays spectacular quantum dynamics wherein the spin angular momentum degree of freedom of one molecule tunnels through 20 units of hbar, with a tunnel splitting of ~ 1 pico eV, or about 1kHz in frequency units. This splitting is about 106 times smaller than the energy bias on a typical molecule in Fe8 crystals due to the dipole-dipole interaction. As a result, tunneling is strongly inhibited by energy conservation, and essentially impossible. The overall relaxation of magnetization is thus exceptionally slow, and understanding it is a challenging problem in classical many-body physics.

We will describe the theoretical model for how we believe Fe8 relaxes, along with Monte Carlo simulations and kinetic equations for the spin and dipolar-field distributions. We apply these approaches to various experimental protocols. The agreement between simulations, kinetic equation, and experiments is very good in most respects, but not so good for ultra long times and ultra-slow phenomena. The problem of how an initially demagnetized sample can be magnetized is particularly interesting and still open, and entails a situation where the magnetization relaxes.

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"Aside stuff as of now…." Or relevant papers?
SMM discussion evolves to SCO discussion.

1. "Single Molecule Magnets on metallic and magnetic surfaces", M. Mannini, et al. (R. Sessoli)
http://www.esrf.eu/files/live/sites/www/files/events/conferences/usersmeeting2011/Abstract_Sessoli_esrf_2011.pdf
2. "Single-molecule Magnet Mn_{12} on graphene", X.-G. Li, J.N. Fry, and H.-P. Cheng, PRB 90 (2014) 125447
http://journals.aps.org/prb/pdf/10.1103/PhysRevB.90.125447
3. "Photomagnetism of iron(II) spin crossover complexes – the *T*(LIESST) approach", J.-F. Létard, J. Mater. Chem. 16 (2006) 2550-2559, http://pubs.rsc.org/en/content/articlepdf/2006/jm/b603473j
4. "The spin state of a molecular adsorbate driven by the ferroelectric substrate polarization", X. Zhang et al. (P.A. Dowben), Chem Commun. 50 (2014) 2255-2257,
http://pubs.rsc.org/en/content/articlepdf/2014/cc/c3cc46892e?page=search

Review aspects of professional behavior and expectations.
https://www.nap.edu/catalog/12192/on-being-a-scientist-a-guide-to-responsible-conduct-in

Week 12	Nov 05	Anupam Garg visit, debriefing. Finish SMM list of "questions" and further discussion?
	Nov 07	SMM – powerpoint slides posted. ***Temperature? Which one: lattice, electron, nuclei?***
Week 13	Nov 12	Individual Meetings, Projects (Intellectual Merit and Broader Impacts finalized)
	Nov 14	Individual Meetings and time for Outreach activities

Course requirements:

One "project", pre-approved by instructor, and classroom presentation (20 min). "Intellectual Merit" (40%)
One outreach "spot" (the elevator speech) or "K-12 activity". "Broader Impacts" (40%)
A one-pager about where you started and where you finished the wild ride. (20%)

Week 14	Nov 19	Presentation 2, 3, 4 (15 min plus 5 min for questions)
	Nov 21	Outreach activities
Week 15	Nov 26	Presentation 5, 6, 7, 8, 1 (15 min plus 5 min for questions)
	Nov 28	No Class, Thanksgiving.
Week 16	Dec 03	Last Day of Class: **Target Date for one-pager about where you started and where you finished the wild ride. (20%) (e.g. What did you learn?)**

AND COMPLETE online course evaluations in your Canvas course menu under GatorEvals tab by using: https://ufl.bluera.com/ufl/

"Students are expected to provide professional and respectful feedback on the quality of instruction in this course by completing course evaluations online via GatorEvals. Guidance on how to give feedback in a professional and respectful manner is available at https://gatorevals.aa.ufl.edu/students/. Students will be notified when the evaluation period opens, and can complete evaluations through the email they receive from GatorEvals, in their Canvas course menu under GatorEvals, or via https://ufl.bluera.com/ufl/. Summaries of course evaluation results are available to students at https://gatorevals.aa.ufl.edu/public-results/."

	Dec 05	No Class, Reading Period

Final Exam Period for this course: 09 Dec 2019 @ 10:00 AM - 12:00 PM (Noon).
There will NOT be a Final Exam,
but ALL GRADED WORK MUST BE COMPLETED and SUBMITTED by NOON on Monday, 09 Dec 2019.