Micro-Nanoscale Energy Transport and Conversion
ME 3295-005 (Class Number 12184) / ME 5895-003 (Class Number 12185)
Tuesday/Thursday 12:30 – 1:45 p.m., Laurel Hall 109

Syllabus

Credits & contact hours: 3 credits. Two 75 minute lectures per week.

Instructor: Prof. Michael T. Pettes
Office: UTEB 354
Email: pettes@engr.uconn.edu
Website: http://pettes.engr.uconn.edu

Time & place: **Lecture:** T/Th 12:30 – 1:45 p.m., LH 109

Instructor office hours: F 10:00 a.m. – 12:00 p.m., UTEB 354

Web page: https://lms.uconn.edu (HuskyCT, login with NetID)

Course description: This course introduces the fundamentals and applications of micro- and nano-scale energy transport. A central theme throughout the course is a parallel theoretical treatment of the transport of various energy carriers including electrons, molecules, phonons, and photons in different applications. The main focuses are (i) theory and experiments of thermal transport in nanomaterials and nanoscale systems and (ii) fundamentals and recent advancements in thermal-to-electrical energy conversion. These topics are essential for advanced research in micro-nano scale heat transfer and are useful for existing and emerging applications in microelectronics, energy conversion, and nanotechnology.

Catalog description: Topics include an introduction into the fundamentals of electron and thermal transport and statistical behavior of energy carriers, theory and experiments of thermal transport in nanomaterials and nanoscale systems, derivation of classical laws and deviation at the nanoscale, and fundamentals and recent advancements in thermal-to-electrical energy conversion.

Prerequisites: PHYS 1502Q[*,†,§] Physics for Engineers II or PHYS 1602Q[‡] Fundamentals of Physics II. MATH 2410Q[*,†,‡,§] Elementary Differential Equations. MSE 2001[†] Introduction to Structure, Properties, and Processing of Materials I, or PHYS 2300[‡] The Development of Quantum Physics, or ECE 3001[§] Electromagnetic Fields and Waves, or ME 3242[*] Heat Transfer. Instructor consent may be granted for special circumstances. *(Note: listed pre-requisite requirement will go into effect in Fall 2016)*

([*]Required course for ME majors, [†]Required course for MSE major, [‡]Required course for PHYS major, [§]Required course for ECE majors)

Text (Required): Chen, Gang, *Nanoscale Energy Transport and Conversion: A Parallel Treatment of Electrons, Molecules, Phonons, and Photons*, (Oxford University Press, 2005), ISBN 9780195159424.

Software (Required): *Mathematica* by Wolfram Research, available free to UConn faculty, staff, and students: http://software.uconn.edu/mathematica/. Students will need to install on their personal/office computer as this software will be used to complete the first homework. The current version is 10.3.

Supplemental Text and Resources (not required): Ashcroft, Neil W., and Mermin, N. David, *Solid State Physics*, (Cengage Learning, 1976), ISBN 0030839939; Kittel, Charles, *Introduction to Solid State*

Physics, 8th ed., (John Wiley & Sons, 2005), ISBN 9780471415268; Chen, Gang, 2012, online material for MIT 2.57 available at http://ocw.mit.edu/courses/mechanical-engineering/2-57-nano-to-macro-transport-processes-spring-2012/index.htm.

Reading: Students are responsible for the assigned material from the course text, whether covered in class or not. Material should be read prior to lectures.

Grading:

	Homework	20 %
	Class participation	10 %
	Midterm exam 1	15 %
	Midterm exam 2	15 %
	Final Project	25 %
	Final exam	15 %
	Bonus Credit	10 %

Important dates:

Monday, February 1, 2016: Last day to add or drop courses without additional signatures. Courses dropped after this date will have a "W" for withdrawal recorded on the academic record.

Monday, March 28, 2016: Last day to drop a course.

Homework: Weekly homework assignments will be due at the beginning of each Tuesday lecture (except for the final homework) and will be graded on the demonstrated level of effort. Homeworks will be printed on 8.5×11 inch paper. The software package *Mathematica* is required for computing and visually representing results. ***All homework problems, including proofs, are to be conducted and handed in using Mathematica (with the exception of ~1 page written assignments).*** Logical thought, assumptions, units, and commenting will be labeled using textual formatting, and all graphs will have axes, units, and plots/legends clearly labeled. Late homework will not be accepted. The one lowest homework grade will be dropped from the final grade.

Exams: Exams will include two mid-terms as well as a comprehensive final exam. Mid-term exams are open book with one double-sided notes sheet allowed (to be stapled to exam). The final exam is open book with three double-sided notes sheets allowed (to be stapled to exam) as well as a calculator. Make-up exams may be scheduled prior to final examinations for students who were previously excused from a mid-term exam due to a verifiable illness or other officially documented circumstance.

Regrading policy: Regrade requests must be submitted in writing on a separate sheet of paper (with the exception of errors in adding up exam points). Do not write on the exam pages or alter the exam in any form. Exams are graded based on a specific set of guidelines and requests to alter these will be denied out of fairness to the class. Legitimate regrade requests will be granted in the case details have been overlooked during the grading process where partial credit has not already been awarded.

Final Team Project: The final project will consist of a 10 page paper (including references and figures) and a 20 minute presentation on a topic relevant to nanoscale thermal transport, quantum confined systems, or nanomaterials for energy conversion and storage. Students will be required to review several key publications of emerging or active research in these areas. Students are required to discuss their proposed topic with and obtain approval from Prof. Pettes prior to the 5 minute topic proposal presentation and 400-word abstract submission on March 1, 2016. The final paper will be 10 pages, 1” margins, 12 point Times New Roman, 1.5 line spacing, and references will include all authors/title/DOI hyperlink. More information is given in the project assignment handout.

Special events: Students are encouraged to attend special events by experts visiting UConn noted in this syllabus. Bonus points of 3.33% for each event will be added to the final grade. ***Only special events listed in this syllabus will be eligible for bonus points.***

In order to receive credit, students must attend the seminar, sign the ME 3295/5895 sign-in sheet, and write a brief (roughly one page) report with three sections discussing

(i) the motivations for the speaker's research,

(ii) significant contributions made by the speaker, and

(iii) remaining challenges or new research areas proposed by the speaker.

Special notes: The University of Connecticut provides upon request appropriate academic adjustments for qualified students with disabilities at the Center for Students with Disabilities (CSD). If you have a documented disability for which you wish to request academic accommodations and have not contacted the CSD, please do so as soon as possible. The CSD is located in Wilbur Cross, Room 204 and can be reached at (860) 486-2020 or at csd@uconn.edu. Detailed information regarding the accommodations process is also available on their website at http://www.csd.uconn.edu, 860-486-2020 (voice), 860-486-2077 (TDD). Inform me if you have CSD requirements.

Observance of university policies: Standard university policies relating to accommodation for students with disabilities, NCAA student-athletes, and to academic misconduct will be followed in this course. Information regarding academic misconduct policies may be found in the "Student Code" available from the Division of Student Affairs, http://www.community.uconn.edu/student_code.html.

Measurement and evaluation: Standard course/instructor evaluations will be administered at the end of this course. The student evaluation of teaching (SET) will be completed online.

Micro-Nanoscale Energy Transport and Conversion
ME 3295-005 (Class Number 12184) / ME 5895-003 (Class Number 12185)
Tuesday/Thursday 12:30 – 1:45 p.m., Laurel Hall 109

Class schedule (subject to periodic revision)

Date	Day	Topic	Chapter	Reading	Homework
Jan. 19	T	Introduction to Nanoscale Transport, Review of Energy Transfer Mechanisms, Introduction to *Mathematica* programming	1	1.1-1.2	
Jan. 21	Th	Kinetic Theory, Thermal Conductivity Measurement Schemes	1	1.3-1.4	
Jan. 22	**F**	**Special Event 1, Gant Science Complex, Physics Building, Room PXXX, 4:00-5:00 p.m.:** **Prof. Jennifer Ogilvie**, Physics, University of Michigan, Ann Arbor, MI. *"Title: Shedding New Light on Photosynthesis"*			
Jan. 26	T	Quantum Concepts	2	2.1–2.3	Set 1 Due
Jan. 28	Th	Introduction to Crystallography	3	3.1	
Feb. 2	T	Electron Energy Levels	3	3.2	Set 2 Due
Feb. 4	**Th**	**No Class, NSF Panel Review**			
Feb. 9	T	Crystal Vibrations and Phonons	3	3.3	Set 3 Due
Feb. 11	Th	Density of States	3	3.4	
Feb. 16	T	Statistical Thermodynamics (Statistical Distributions)	4	4.1	Set 4 Due
Feb. 18	Th	Specific Heat	4	4.2–4.3	
Feb. 23	**T**	**Midterm Exam 1 (Chapters 1–3, in class, open book, 1 double sided notes page)**			
Feb. 25	Th	Wave Propagation	5	5.1	
Mar. 1	T	Team Project Proposals – 5 min. ea.			Set 5 & Project Abstracts Due
Mar. 3	Th	Interfacial Transport	5	5.2–5.4	
Mar. 8	T	Quantum Conductance	5	5.5	Set 6 Due
Mar. 10	Th	Coherence Effects	5	5.6	
Mar. 15	**T**	**No Class, Spring Recess**			
Mar. 17	**Th**	**No Class, Spring Recess**			
Mar. 22	T	Non-Equilibrium Effects Boltzmann Transport Equation	6	6.1	Set 7 Due
Mar. 24	Th	Scattering Theory I	6	6.2	
Mar. 29	**T**	Scattering Theory II	6	6.2	Set 8 due
~~Mar. 31~~	~~Th~~	~~Thermoelectric Transport I~~	~~6~~	~~6.3~~	
Apr. 1	**F**	**Special Event 2, Gant Science Complex, Physics Building, Room P038, 4:00-5:00 p.m.:** **Prof. David Kaiser**, Physics, Massachusetts Institute of Technology, Cambridge, MA. *"Title: Einstein's Legacy: Studying Gravity in War and Peace"*			
Apr. 5	T	**Midterm Exam 2 (Chapters 4–6.2, in class, open book, 1 double sided notes page)**			

Apr. 7	Th	Thermoelectric Transport II	6	6.3	
Apr. 8	**F**	**Special Event 3, Pharmacy/Biology Bldg. PBB 131, 2:30-3:30 p.m.:** **Prof. Xianfan Xu**, Mechanical Engineering, Purdue University, West Lafayette, IN. *"Title: TBA"*			
Apr. 12	T	Thermal Conductivity I	6	6.3	Set 9 due
Apr. 14	Th	Presentation Day 1 – 20 min. ea.			
Apr. 19	T	Presentation Day 2 – 20 min. ea.			Final Papers Due
Apr. 21	Th	Presentation Day 3 – 20 min. ea.			
Apr. 26	T	Presentation Day 4 – 20 min. ea.			
Apr. 28	Th	Thermal Conductivity II, End of course review	6	6.3	Set 10 due
May 2-7	Day	**Final Exam, (Ch. 1–6, open book, 3 double sided notes pages) ← Verify with registrar**			

Micro-Nanoscale Energy Transport and Conversion
ME 3295-005 (Class Number 12184) / ME 5895-003 (Class Number 12185)
Tuesday/Thursday 12:30 – 1:45 p.m., Laurel Hall 109

Homework Sets, Spring 2016 (subject to periodic revision)

Set Number	Assigned Homework Problems: All problems to be solved using *Mathematica*, including derivations. Use the commenting notation to discuss your rationale as you progress through the problem. Print out your .nb file and email a copy to pettes@engr.uconn.edu.
1	1) Complete the *Introduction to Mathematica* notebook posted onto HuskyCT. Print your solutions. 2) Chen 1.7. Plot $k_B T$ as a function of temperature to 1000 K. 3) Read Feynman, Richard P., "There's plenty of room at the bottom," *Engineering and Science* **23**, 22–36 (1960). http://resolver.caltech.edu/CaltechES:23.5.1960Bottom and Toumey, Christopher "Plenty of room, plenty of history," *Nature Nanotechnology* **4**, 783–784 (2009). http://dx.doi.org/10.1038/nnano.2009.356. Write a roughly 1 page summary (Times New Roman 11 pt, 1.5 spacing, 1" margins) discussing the message of Feynman's paper and the commentary by anthropologist Chistopher Toumey**.**
2	1) Chen 1.15. Hint: see section 1.5.2 beginning on page 29. 2) Calculate and plot the thermal conductivity of air inside of an enclosure of diameter *D* as a function of pressure *P* at temperature *T*=300K. Plot for *D*=1/4 inch, 1 inch, and 1 m. Use the range for pressure 10^{-12} mbar $\leq P \leq$ 10 atm. Put all plots on the same graph and design the graph to be intelligible. 3) The 2010 Nobel Prize in Physics was awarded to Andre Geim and Konstantin Novoselov of the University of Manchester *"for groundbreaking experiments regarding the two-dimensional material graphene."* http://www.nobelprize.org/nobel_prizes/physics/laureates/2010/. View Andre Geim's 2010 Nobel Lecture, "Random walk to graphene" http://www.nobelprize.org/nobel_prizes/physics/laureates/2010/geim-lecture.html and write a roughly 1 page summary (Times New Roman 11 pt, 1.5 spacing, 1" margins) discussing the messages of his lecture. Also, thin graphitic carbon has been around for many decades, comment on what Geim & Novoselov published that lead to them being recognized as Nobel Laureates?
3	1) Chen 2.1. Plot the frequency-wave vector relationship for the laser with your solution in the same plot. 2) Chen 2.2. 3) The 2011 Nobel Prize in Chemistry was awarded to Dan Shechtman of Technion *"for the discovery of quasicrystals."* http://www.nobelprize.org/nobel_prizes/chemistry/laureates/2011/. View Dan Schechtman's 2011 Nobel Lecture, "The discovery of quasi-periodic materials," http://www.nobelprize.org/nobel_prizes/chemistry/laureates/2011/shechtman-lecture.html and write a roughly 1 page summary (Times New Roman 11 pt, 1.5 spacing, 1" margins) discussing the message of his lecture. Comment on why 5-fold symmetry was forbidden in periodic structures and what Shechtman did to prove his results indeed could be attributed to a new class of crystal symmetry.

4	1) Chen 3.2. 2a) Chen 3.8. 2b) What are the zone center (k=0) and zone boundary ($k=\pi/a$) frequencies in terms of M_1, M_2, and spring constant K? 2c) Using dummy values for mass and interatomic force constants, what happens for the cases $M_1=M_2$, $M_1=0.5M_2$, and $M_1=0.1M_2$? Make three plots, one each for spring constants K, 2K and 10K. 3a) Chen 3.10. Plot the dispersion $E(k_x, l, n)$ and plot the density of states per unit length L_x, $D(E)$, both up to the 10^{th} energy level. For effective mass, do not assume constant m^*. Use representative values for Bismuth, $m_x^*=0.00597m_0$, $m_y^*=1.33m_0$, $m_z^*=0.0114m_0$. 3b) Now plot both $E(k_j, l, n)$ and $D(E)$ with confinement in the x-z plane ($L_x=L_z$=50 Å), and with confinement in the x-y plane ($L_x=L_y$=50 Å). Plot these together with your results from part (a), i.e. you will have have three plots for each graph, corresponding to quantum wires grown along light (x), medium (z), and heavy (y) electron transport directions. Problem 3 due with HW #5
5	1) Chen 3.12. Using dummy values for mass and interatomic force constants, make two plots, one showing the density of states for M, 2M, and 10M using a fixed K, and another plot showing density of states for K, 2K, and 10K using a fixed M. 2) Chen 4.11. <-- This problem is no longer due. 3) Chen 4.13. Using dummy values for mass and interatomic force constants, make two plots, one showing the density of states for M, 2M, and 10M using a fixed K, and another plot showing density of states for K, 2K, and 10K using a fixed M.
6	1) Chen 5.11. 2) Chen 5.23. Prove and plot both the dispersion and the group velocity within the first Brillouin Zone.
7	1) Read the following papers on quantum thermal conductance and discuss their major conclusions (~ 1 page, Times New Roman 11 pt, 1.5 spacing, 1" margins), specifically, what are the assumptions/requirements leading to the quantum of thermal conductance g_0. Schwab, K., Henriksen, E. A., Worlock, J. M., and Roukes, M. L., "Measurement of the quantum of thermal conductance," *Nature* **404**, 974–977 (2000). http://dx.doi.org/10.1038/35010065. Maynard,R. & Akkermans,E. "Thermal conductance and giant fluctuations in one-dimensional disordered systems," *Phys. Rev. B* **32**, 5440–5442 (1985). http://dx.doi.org/10.1103/PhysRevB.32.5440. 2) Given the phonon dispersions of bulk silicon and a silicon nanowire in HuskyCT, plot the ballistic thermal conductance as a function of temperature for the acoustic phonon branches along with the quantum thermal conductance for these branches. At what temperature does the conductance begin to diverge? Would you expect this given the theory and experimental results of the above reports?

8	1) Chen 6.4. 2) Chen 6.5.
9	1) Chen 6.14.
10	1) Given the phonon dispersion of graphene, develop the appropriate modeling parameters in a Debye/Quadratic acoustic polarization model. Derive an expression for the specific heat and thermal conductivity of graphene considering boundary (1 nm, 100 nm, 1 μm, 1mm) and natural isotopic scattering.

Micro-Nanoscale Energy Transport and Conversion
ME 3295-005 (Class Number 12184) / ME 5895-003 (Class Number 12185)
Tuesday/Thursday 12:30 – 1:45 p.m., Laurel Hall 109

Final Team Project, Spring 2015 – Due in class Tuesday, April 19

Project Topic: The final project will consist of a 10 page paper (including references and figures) and a 20 minute presentation on a topic relevant to nanomaterials for energy conversion and storage, nanoscale thermal transport, or quantum confined systems.

Abstract and Overview Presentation (Due Tuesday, March 1): Teams will prepare a 5 minute presentation to introduce the topic of their final project using the assigned powerpoint template. Teams will also hand in a print copy of their project title and abstract. The abstract is limited to 400 words. Format is 1" margins, 11 point Times New Roman, 1.5 line spacing, and references including all authors/title/DOI hyperlink. Example:

[25] B. Radisavljevic, A. Radenovic, J. Brivio, V. Giacometti, and A. Kis, "Single-layer MoS_2 transistors," *Nat. Nanotechnol.* **6**, 147 (2011). http://dx.doi.org/10.1038/nnano.2010.279

Students are required to discuss their proposed topic with and obtain approval from Prof. Pettes prior to the 5 minute topic proposal presentation on 3/1.

Paper (Due Tuesday, April 19): The final project will consist of a 10 page paper (including references and figures). Students will be required to review several ***key and current*** publications of emerging or active research in one of these areas with the following major sections:

1. Title, Authors, and Abstract (400 word maximum abstract)
2. Introduction
3. State of current research
4. Conclusion and Outlook
5. References

Students are encouraged to read important review articles for tips on effective ways to prepare a review, e.g.: M. Z. Hasan and C. L. Kane, "Colloquium: Topological insulators," *Rev. Mod. Phys.* **82**, 3045 (2010). http://dx.doi.org/10.1103/RevModPhys.82.3045, and A. A. Balandin, "Thermal properties of graphene and nanostructured carbon materials," *Nat. Mater.* **10**, 569 (2011). http://dx.doi.org/10.1038/nmat3064.

Presentation (in class, April 14 – 26): Each team will present a 20 minute presentation of the work discussed in their paper utilizing and expanding upon the overview presentation sections.

Teamwork: All team members will be required to contribute to their team's efforts, including abstract, overview presentation, final paper preparation, and final presentations. Teams are assigned on the following page.

Evaluation: The evaluation of the final project will be based on the initial abstract (5%), overview presentation (5%), final paper (60%) and the project presentation (30%).

Micro-Nanoscale Energy Transport and Conversion
ME 3295-005 (Class Number 12184) / ME 5895-003 (Class Number 12185)
Tuesday/Thursday 12:30 – 1:45 p.m., Laurel Hall 109

Final Project Team Assignments, Spring 2016

Presentations = 20 minutes + 5 minutes for questions per group
Papers are due Tuesday, April 19, 2016 in class for all groups

Presentation Day 1 – Thursday, April 14, 2016		
Group 1, 12:30-12:55 p.m.	**Group 2, 12:55-1:20 p.m.**	**Group 3, 1:20-1:45 p.m.**
Altamura, Daniel John	Belke, Will Joseph	Choi, Alexander Youngsoo
		Carter, Aliya Danielle
Presentation Day 2 – Tuesday, April 19, 2016		
Group 4, 12:30-12:55 p.m.	**Group 5, 12:55-1:20 p.m.**	**Group 6, 1:20-1:45 p.m.**
Choudhry, Usama Ahmed	Kline, Bradley Paul	Manzolillo, Samuel Robert
Dusoe, Keith		
Presentation Day 3 – Thursday, April 21, 2016		
Group 7, 12:30-12:55 p.m.	**Group 8, 12:55-1:20 p.m.**	**Group 9, 1:20-1:45 p.m.**
Mosher, Andrew Davis	Seymour, Casey Sarah	Sweeney, Shawn Alexander
	Steffes, James Joseph	Spyek, John
Presentation Day 4 – Tuesday, April 26, 2016		
Group 10, 12:30-12:55 p.m.	**Group 11, 12:55-1:20 p.m.**	**Group 12, 1:20-1:45 p.m.**
Twarog, Kyle E	Webster, Justin Paul	Wilcox, Shane Ervin