

## Physics Department Senior Design Project Proposal

Project Mentor: Prof. Lincoln Carr, 303 273 3759, lcarr@mines.edu; Prof. Mark Lusk, 303 273 3675, mlusk@mines.edu

Project Title: Computational Physics: Nanoengineering of Graphene

Project Type: [ X ] Team; Number of students 2 [ X ] Honors

### Objective

(What is the science and/or engineering in this project?)

The age of silicon electronics is shortly coming to a close, which means the end of Moore's Law (computing power doubles every 1 ½ years). One excellent candidate for a replacement is graphene, a solid planar form of carbon. In this project, students will study nano-engineered graphene with two sets of simulation methods: (1) exact diagonalization, or a full quantum simulation; (2) density functional theory (DFT), approximation methods which are used for all kinds of advanced materials in condensed matter physics, as well as other fields. The goal is to compare the properties of the full quantum solution, including entanglement and electron-electron correlations, to the DFT approximations. The reason we do this is that DFT can be extended to hundreds of carbon atoms, while exact diagonalization is restricted to very small systems. In addition, nanoengineered graphene of this form can be a quantum dot, an "artificial atom" which confines electrons.

### Prior Background

(What is the history of your involvement with this topic, including previous student projects?)

Prof. Lusk and Prof. Carr have spent the last year working intensively on this project. A number of students in Prof. Lusk's group have expertise

### Student Expectations

(What are the deliverables (in addition to the lab notebook and reports) for the two-semester project?)

One student will adapt existing exact diagonalization Matlab code of a honeycomb lattice to include defects. The other will work with density functional theory in Materials Studio. Both students will learn about density functional theory, quantum information theory, and relevant condensed matter physics of 2D lattices. Students will work together to compare and contrast results from these two methods. Students will present correlation and entanglement properties of "defect domains," i.e., sections of graphene nano-engineered to have particular mechanical, electrical, thermal, and chemical properties.

Specifically: Students will determine to what extent entanglement from exact diagonalization is contained in the DFT simulations. I.e., to what extent does method (2) represent the complete physics of method (1). They will do this first for simple graphene, as a warm-up, then move on to nano-engineered graphene-based materials. They will work their way up from single "blisters" or defect domains to arrays of such domains, called meta-crystals. To answer these questions they will apply specific quantum measures, such as von Neumann entropy, to the output of their simulations.

This work is expected to lead to a publication.

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This project is suitable for extension to an MS thesis if so desired.

Both students will be required to attend theoretical physics seminar (PHGN401); the DFT student will be required to attend the Lusk group meeting, while the exact diagonalization student will be required to attend the Carr team meeting (quantum team), for a total of two hours per week each. Each student will present his/her work in theoretical physics seminar once during the year.

### Supervision Plan

(Who will be directly interacting with the student(s), you, a post-doc, grad students, or others?)

The students will work with Prof. Carr, Prof. Lusk, MS student Sean Santos, and other students in the group of Prof. Lusk. The student working with Materials Studio will be trained in that program primarily by PhD student Abram van der Geest (Bram).

### Resources

(What equipment, algorithms, and facilities are available, and what will be assembled as part of the project?)

Use of computers in undergraduate physics area suffice. Extant C code compiles already on these machines and has been used previously for other projects.

### Technical References

(Identify a few key starting points for the student(s); journal citations, prior reports, instruction manuals, etc.)

Mark T. Lusk and L. D. Carr, "Nano-Engineering Defect Structures on Graphene," Phys. Rev. Lett. v. 100, p. 175503 (2008)

and references therein