

Managing the Partnership I: From BS and MS Perspective

W. M. Keck Computational Materials Theory Center (CMTC)
California State University Northridge

and

Princeton Center for Complex Materials (PCCM)
Materials Research Science and Engineering Center (MRSEC)



Nicholas Kioussis

California State University
Northridge



NSF PIs PREM
14 September, 2012

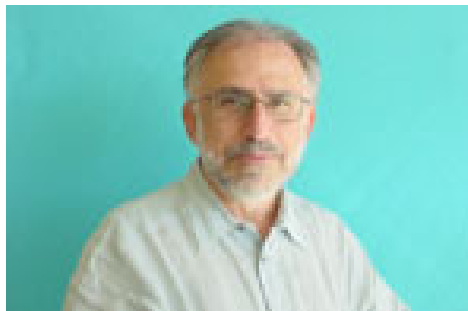
Objective of PREM

Expand/strengthen research/education of W. M. Keck CMTC at CSUN, a Hispanic-serving institution, by forming a formal and long-term collaborative relationship with the MRSEC PCCM

Goals – Vision

- Foster multidisciplinary and innovative research in computational materials science
- Educate and train students in cutting-edge computational materials science (*New curriculum development*)
- Stimulate/develop strong industrial-university-national laboratory partnerships
- Increase recruitment, retention, and degree attainment by members of groups underrepresented in materials research
- Outreach (*High-School Teacher Computational Materials Camp; Distinguished Lecture Series, etc.*)
- Expand to soft condensed matter and experimental materials science

Faculty at W. M. Keck CMTC



Nicholas Kioussis



Gang Lu



Donna Sheng

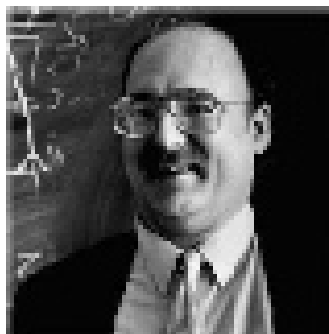
Faculty at PCCM- MRSEC



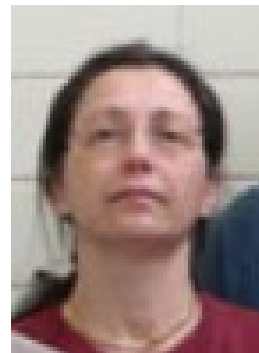
Emily Carter



Roberto Car



Duncan Haldane



A. Selloni



Weinan E



Nai-Phuan Ong

Faculty exchange visits between PCCM and CSUN

1. Nick Kioussis (CSUN) to PCCM	2006	(research)
2. Gang Lu (CSUN) to PCCM	2006	(research)
3. Roberto Car (PCCM) to CSUN	2007	(research)
4. Gang Lu (CSUN) to PCCM	2007	(research)
5. Nick Kioussis (CSUN) to PCCM	2007	(research)
6. Emily Carter (PCCM) to CSUN	2007	(admin, research)
7. Kioussis and Car (at KITP)	2008	(research)
8. Donna Sheng and N. P. Ong (at KITP)	2008	(research)
7. Donna Sheng (CSUN) and Duncan Haldane (at KITP and at Princeton)	2009	(research)
8. Gang Lu (CSUN) to PCCM	2009	(research)
9. Jason Petta (PCCM) to CSUN	2009	(panel review)
9. Donna Sheng (CSUN) to PCCM	2009	(summer research)
10. Kioussis and Car (at KITP)	2010	(research)
11. Annabella Selloni (PCCM) to CSUN	2011	(research)
12. Kioussis, Lu, and Selloni, Ong	2011	(research)
13. Annabella Selloni (PCCM) to CSUN	2011	(research)
14. Daniel Steinberg (PCCM) to CSUN	2011	(education/outreach)

IMPACT OF **PCCM –MRSEC** ON RESEARCH

- ✓ The research thrusts coupled strongly to several corresponding thrusts in the Princeton MRSEC
- ✓ Elevate and advance our research and education scopes to achieve national competitiveness
- ✓ Publish in high-impact journals
- ✓ Expand our research in new areas and develop novel techniques for (1) multiscale modeling to study more complex physical phenomena, (2) strongly correlated electron systems, and (3) spin transport in magnetic tunnel junctions

CSUN and PCCM faculty

- 1) Q. Peng, X. Zhang, L. Hung, E.A. Carter and G. Lu, “Quantum simulation of materials at micron scales and beyond”, *Phys. Rev. B* **78**, 054118 (2008).
- 2) G. Wu, G. Lu, C.J. Garcia-Cervera, and W. E, “Density-gradient-corrected embedded atom method”, *Phys. Rev. B* **79**, 035124 (2009).
- 3) Y.H. Tang, N. Kioussis, A. Kalitsov, W.H. Butler, R. Car, “Influence of asymmetry on bias behavior of spin torque”, *Phys. Rev. B* **81**, 054437 (2010).
- 4) Lijun Zhu, R. Ma, L. Sheng, M. Liu, and D. N. Sheng, “Universal thermoelectric effect of Dirac fermions in graphene”, *Phys. Rev. Lett.* **104**, 076804 (2010).
- 5) H. Wang, D.N. Sheng, and F.D.M. Haldane, “Particle-hole symmetry breaking and the $\nu=5/2$ fractional quantum Hall effect”, *Phys. Rev. B* **80**, 241311 (2009).
- 6) Y.H. Tang, N. Kioussis, A. Kalitsov, W.H. Butler, R. Car, “Controlling the Nonequilibrium Interlayer Exchange Coupling in Asymmetric Magnetic Tunnel Junctions”, *Phys. Rev. Lett.* **103**, 057206 (2009).
- 7) Q. Peng, X. Zhang, C. Huang, E.A. Carter and G. Lu, “Quantum mechanical study of solid solution effect on dislocation nucleation during nano-indentation”, *Modeling Simulation Mater. Sci. Eng.* **18**, 075003 (2010).

Education

- Promote accessibility of frontier research/education experience in multidisciplinary computational science to students from underrepresented groups
- Expand and strengthen the existing curriculum in materials science in the Physics Department via the development of a sequence of new courses.

Impact of NSF-PREM to students

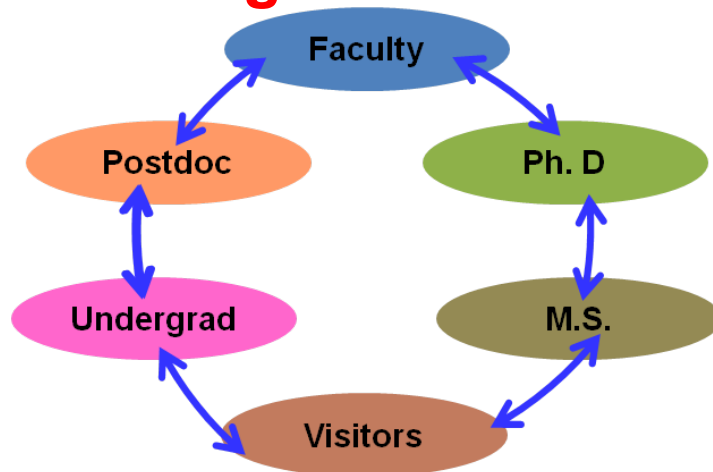
✓ **Publications** (\approx 14-17 % with undergraduates/MS students)

1. Srevatsan Muralidharan, [Raika Khodadad](#), [Ethan Sullivan](#), and Mikko Haataja, *Multilayer thin film growth on crystalline and quasicrystalline surfaces: A phase-field crystal study*, Phys. Rev. **B 85**, 245428 (2012).
2. J. Li, [J. Gayles](#), Nicholas Kioussis, Z. Zhang, C. Grein, and F. Aqariden, *Ab initio studies of the unreconstructed polar (111) CdTe surface*, J. Electronics Materials (in press, 2012).
3. Luis Agapito, [Jacob Gayles](#), [Christian Wolowiec](#), and Nicholas Kioussis *Aviram-Ratner rectifying mechanism for DNA base-pair sequencing through graphene nanogaps*, J. of Nanotechnology, **23** 135202 (2012).
4. Alexandros Chremos, [Kelly Margaritis](#) and Athanassios Z. Panagiotopoulos, “*Ultra thin films of diblock copolymers under shear*”, Soft Matter **6**, 3588-3595 (2010).

Impact of NSF-PREM to students

- ✓ **Exposure to research/education at**
 - ❖ MRSEC Princeton University (9 weeks REU summer visits)
 - ❖ Industries (EPIR, INTEL)
 - ❖ National Laboratories (US Air Force, Livermore)

✓ **Mentoring and Role Model**



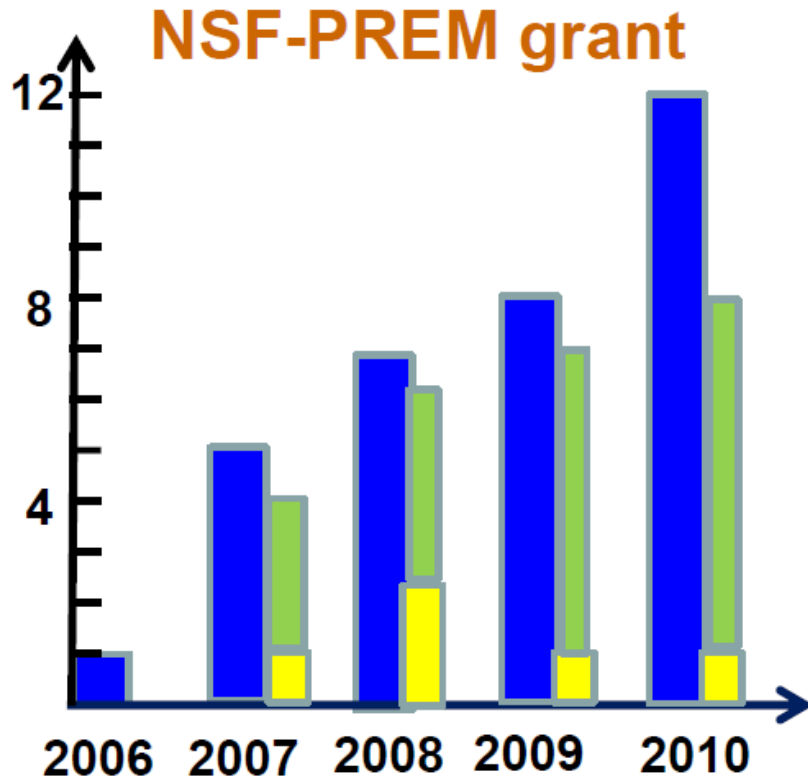
Weekly group meetings, seminars,

- ✓ **REU student visits to Princeton reinforced strong work ethic**

Benefits of NSF-PREM to students

- ✓ **Presentations in conferences and workshops** (APS, MRS, Stanford, UC Berkley, Conference for African American Researchers in the Mathematical Sciences)
- ✓ **Presentations in the annual High-School Teachers Computational camps for nanotechnology tool kits**
- ✓ **REU students mentoring middle school students in PUMA**
- ✓ **PREM students serve as ambassadors to local high schools**
- ✓ **PREM students serve as mentors to high-school students**
 - **summer interns** (K. Choudhary (2009) accepted at Princeton; Shoba Paul (2010) applying to UC Berkley and Caltech)

Publications



total
PRL
PRB

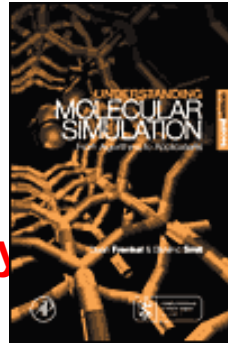
≈ 14-17 % with
undergraduates/MS
students

> 25 total publications annually

Development of a sequence of novel courses (Spring semester)

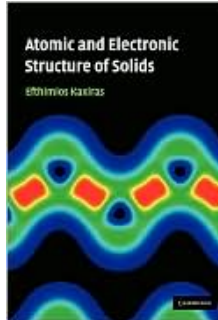
I. Atomistic Simulation of Materials (596 CMTA)

Molecular Dynamics and Monte Carlo calculations of structural and thermal properties of materials. **Text Book: Understanding Molecular Simulation by Frenkel and Smit.**



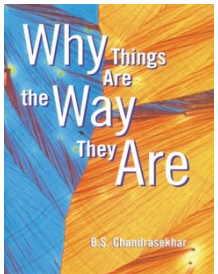
II. Electronic Structure Calculations (596 CMTB)

Tight Binding; Density Functional approach; Pseudopotentials; Plane Waves; BZ k-point sampling, energy cut offs, etc. Hands on experience with VASP (structural, magnetic and optical properties of bulk and surfaces)



III. Effect of Strong Electron Correlations (596 CMTC)

Magnetic order; spin wave theory; spin-liquid behavior in frustrated magnetic system; Mott-insulator and quantum phase transition in Hubbard model



IV. Special Lectures For Seniors and Juniors

Crystals, Lattice symmetry, wave-particle duality, wave functions

UNIX

Visualization software (XMGR, VASPView)

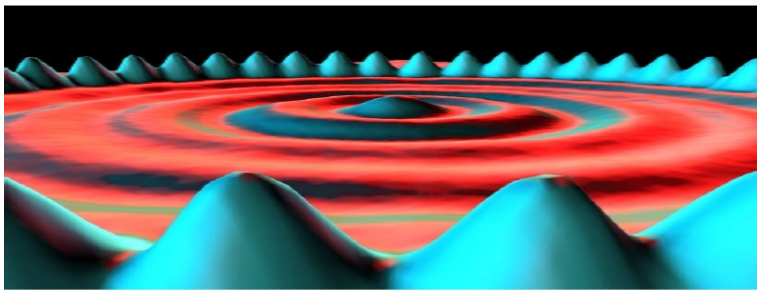
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Grand Challenges

- Development of work ethic
- Wide range of educational background of undergraduate students (Freshmen to Senior)
- Lack of learning tools to attack specific problems (from courses to computational techniques) **(Solution: development of a special sequence of courses)**
- Insufficient time to conduct research for 1st year MS students
- Difficulty in retaining physics majors due to lack of preparation **(Possible solution: Recruitment of non-physics majors, i.e., chemistry, engineering, etc.)**

Outreach

- Difficulty in recruiting physics majors
- Difficulty in retaining physics majors



California State University
Northridge



Nanotechnology Workshop for Teachers at California State University Northridge

May 10 and May 17, 2008 , April 2010, April 2012

Purpose

One of the thrusts of PREM is to form a formal and long-term collaborative relationship with the Los Angeles Unified School District in Nanotechnology.

Two-day workshop to explore nanoscience and nanotechnology. Topics included: Effects of size and scale; unusual properties at the nanoscale; tools for measuring and manipulating atoms and molecules; examples of applications of nanoscience; ways to bring nanotechnology into their middle and high school classes.

- Certificate of attendance
- CD with workshop materials

Taft, Reseda, Panorama, Birmingham,
Northridge Academy, Valley Alternative,
Magnet

Nanotechnology Academy **NSF PIs PREM**
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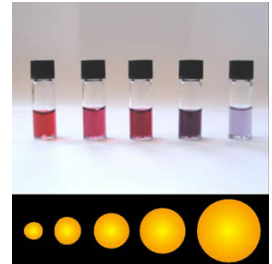
Lectures of PREM students on Nanotechnology Education Kits to

- High-School Teachers
- High-School Students



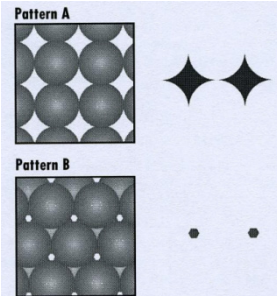
- **Size Dependent Properties of Materials (Jacob Gayles)**

- Chemical and physical properties depend the size
- Changing size of nanoparticles affects the color



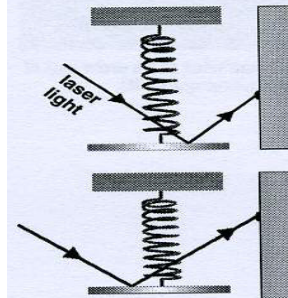
- **Fabricating Nano-Sized Objects (Sergio Orozco)**

- Introduce Nanolithography and compare serial and parallel fabrica
- Model Nanosphere Lithography and simulate patterns of nanoparticles



- **Amplifying the Nanoscale to the Macroscale (Eric Sanchez)**

- Investigate a way to amplify nanoscale detection to our macroscale awareness.
- Model two essential parts of an AFM using the spring force and a laser.



CONFERENCES



Energy Harvesting---From Fundamentals to Devices

March 25 - 27, 2008

Chairs

Harry Radousky

Lawrence Livermore National Laboratory

James Holbery

Pacific Northwest National Laboratory

Bob O'Handley

Massachusetts Institute of Technology

Nicholas Kioussis

California State University-Northridge

Kavli Institute for Theoretical Physics, UC Santa Barbara

Low Dimensional Electron Systems

Coordinators: Herb Fertig, Donna Sheng, Kun Yang



Scientific Advisors: Sankar Das Sarma, Jim Eisenstein, Amir Yacoby

January 20, 2009 - June 12, 2009

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EXPANSION OF NSF PREM

EXPANSION OF PREM FACULTY



Igor Beloborodov (09)
(Condensed Matter Theory)



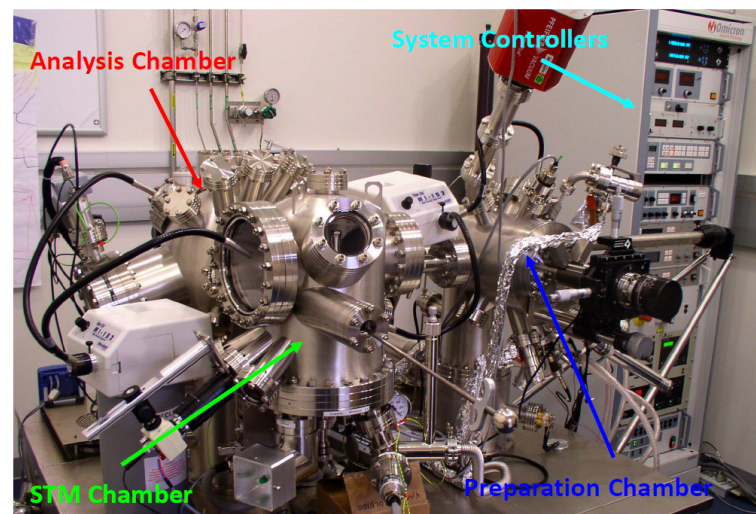
Jussi Eloranta (06)
Chemistry

Li Gao (12)

(Condensed Matter Experiment)

Ultra High Vacuum Scanning Tunneling Microscope System

**Strengthen/expand Experimental
Facilities in Nanotechnology
Surface Analysis/Processing Facilities**



External Funding

Over \$ 1,500,000 annually

- NSF-PREM
- NSF
- DOE
- US ARMY
- US AIR FORCE
- US Navy
- NIH
- DARPA
- DTRA
- NATIONAL RECONNAISSANCE OFFICE
- INTEL
- SIVANANTHAN LABS
- EPIRSENSORS

Collaborations

Princeton, Harvard, UCSB, UCLA, USC, Brown, U. Alabama, Tshinghua U, Hong Kong U. Sci. Tech.

Lawrence Livermore Natl Laboratory, Naval Research Laboratory, Argonne National Lab, Los Alamos Natl. Lab, Intel, EPIRSENSORS

University Support

- ✓ **50 % reassigned time** (Department, College, Provost)
- ✓ **Space infrastructure (\$500 K - renovation of 5,000 square feet for W. M. Keck CMTC)**
- ✓ **System Administrator; Electronics technician**
- ✓ **\$300 to \$600 K start up funds for recent hires**
- ✓ **University matching funds (25% for NSF-PREM)**

Future Thrusts – Sustaining-expanding PREM

