PREM

Multidisciplinary Research and Education in Computational Materials Science

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)

https://www.csun.edu/nsfprem/

NSF

California State University Northridge

Princeton Center for Complex Materials

Objective of PREM

Expand and strengthen the research/educational activities of W. M. Keck CMTC at CSUN, a Hispanic-serving institution, by forming a formal and long-term collaborative relationship with the Princeton Center for Complex Materials (PCCM), a Materials Research Science and Engineering Center (MRSEC).

W. M. Keck CMTC

- **Foster multidisciplinary and innovative research in computational materials science**
- **Educate and train students in cutting-edge computational materials science**
- **Stimulate/develop strong industrial-university-national laboratory partnerships**
- **Increase recruitment, retention, and degree attainment by members of groups underrepresented in materials research**

Faculty at W. M. Keck CMTC

Nicholas Kioussis

Gang Lu

Donna Sheng

Faculty at PCCM- MRSEC

Emily Carter

Roberto Car

Duncan Haldane

Annabella Selloni

Weinan E

Undergraduate students

Jacob Gayles

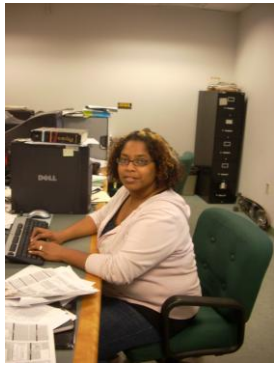
Eric Sanchez

Sergio Orozco

M.S. students

Chris Wolowiec

Rajiv Uttamchandani



Courtney Sams

Ph.D. students

Benjamin Ramirez

Postdoctoral Fellows

Qing Peng

Hao Wang

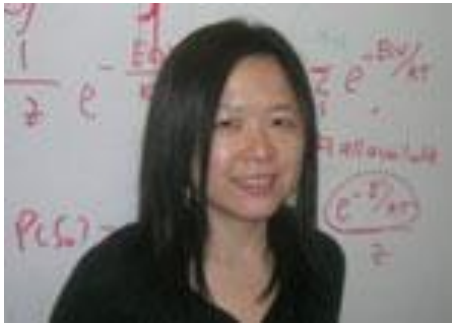
Tina Tang

Luis Agapito

Graduated Members

M.S. students

Michael Vargas
(NWAA Labs)



Mu-Chin(Amy) Huang

Jaime Osorio
(High School Teacher)

Ph.D. students

Xu Zhang

Ioannis Theodonis

Successful student stories

J. Thevenot (U. Arizona)

A. Lee, D. Swearingen (Ohio State U.)

R. Hemker, R. Zhandi (UCLA)

J. Pruet (Yale, currently at LLNL)

S.H. Park (U. of Chicago)

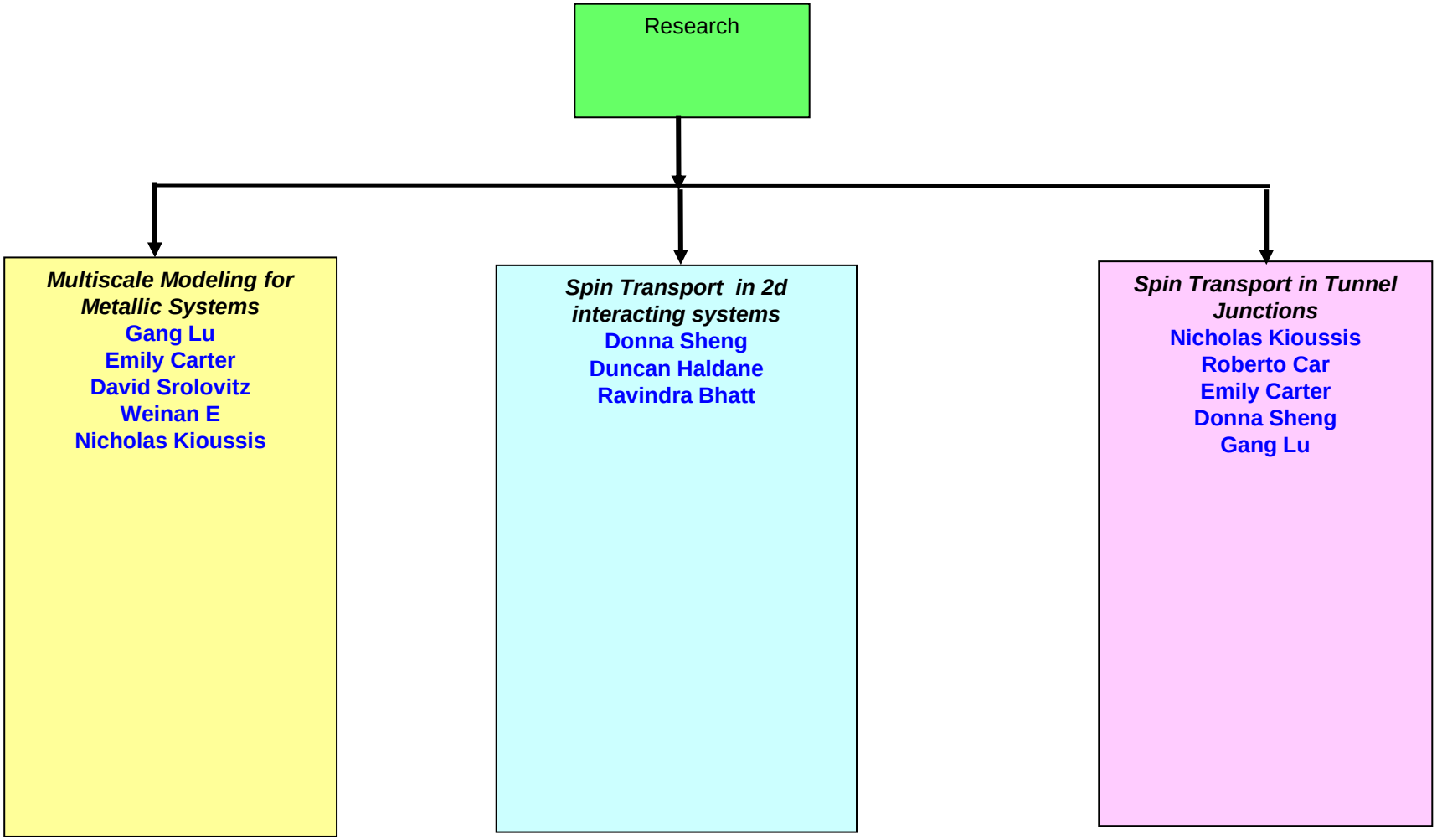
H. Watanabe (Stanford)

H. Yu (UCI)

M. Tovar (UCR)

G. Lu (Ph.D at CSUN, postdoc at Harvard, faculty at CSUN, Co-PI in PREM)

R. Zhandi (MS at CSUN, Ph.D. UCLA, postdoc at MIT, faculty at UCR)


Research
Multiscale Modeling for Metallic Systems
Gang Lu
Emily Carter
David Srolovitz
Weinan E
Nicholas Kioussis
Spin Transport in 2d interacting systems
Donna Sheng
Duncan Haldane
Ravindra Bhatt
Spin Transport in Tunnel Junctions
Nicholas Kioussis
Roberto Car
Emily Carter
Donna Sheng
Gang Lu

W. M. Keck CMTC Infrastructure

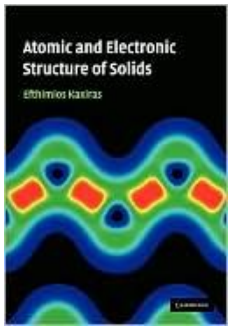
- 32-processor SGI Origin3800 & 16-processor SGI Origin2400 parallel servers
- 40-node dual processor AMD Opteron 2.2GHZ cluster
- 20-node dual processor AMD Opteron 2.2 GHz cluster
- 16- processor Compaq DEC Alpha parallel server
- Dual processor SGI octane and a SGI O2 workstation

Educational Activities

Sequence of novel courses (NSF-PREM)

I. Atomistic Simulation of Materials

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

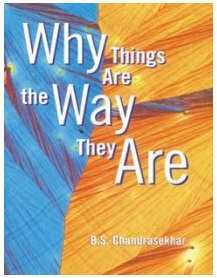
Tight Binding; Density Functional approach; Pseudopotentials; Plane Waves; BZ k-point sampling, energy cut offs, etc. Hands on experience with VASP (structural, magnetic and optical properties of bulk and surfaces)

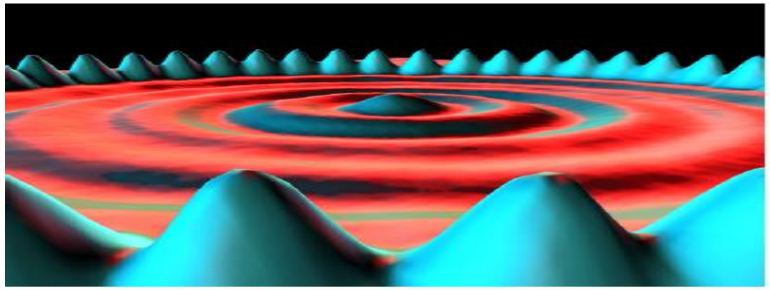
III. Effect of Strong Electron Correlations

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





California State University Northridge

Nanotechnology Workshop for Teachers at California State University Northridge

May 10 and May 17, 2008 - April 2010

Purpose

One of the thrusts of PREM is to form a formal and long-term collaborative relationship with the Los Angles 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**

High Schools

Taft, Reseda, Panorama

High-School Summer Internships

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

EXPANSION OF PREM

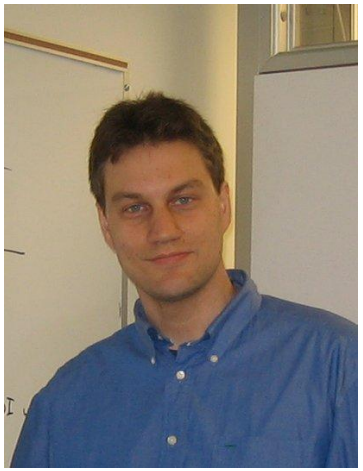
RECENT FACULTY HIRES

Igor Beloborodov

(Condensed Matter Theory)

Yohannes Shiferaw

(Soft Condensed Matter)



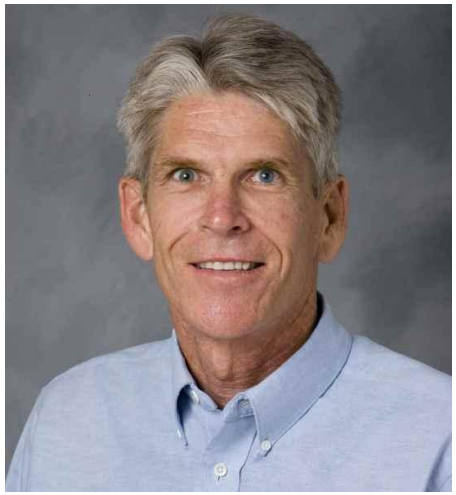
Henk Postma

(Condensed Matter Experiment)

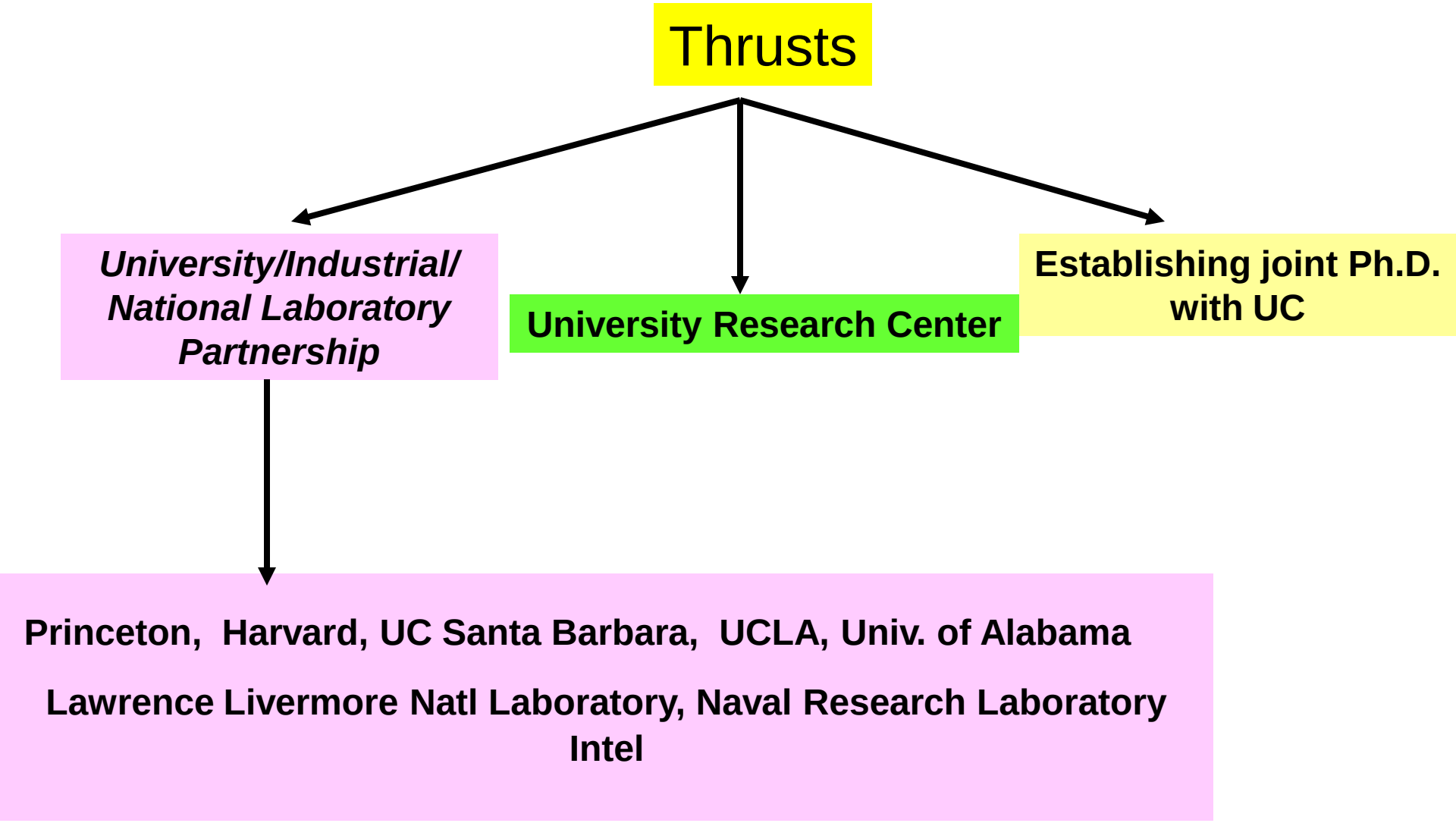
Jussi Eloranta

Simon Garrett

Maria D'Orsogna



Dale Conner


Thrusts
University/Industrial/ National Laboratory Partnership
University Research Center
Establishing joint Ph.D. with UC
Princeton, Harvard, UC Santa Barbara, UCLA, Univ. of Alabama
Lawrence Livermore Natl Laboratory, Naval Research Laboratory
Intel

2004-2008 External Funding
$ 3,502,765

NSF-NIRT (UCLA)	US Army	DOE	NIH
DOE (SciDAC)	DOE	Intel	

DARPA; NASA (URC); NSF (CREST)

Other 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
- $200 - $600 K start up funds for recent hires
- University matching funds (25% for NASA and CREST)
- Hire of additional 5 faculty positions