TEMPLE UNIVERSITY

College of Science and Technology

Temple University's Center for Computational Design of Functional Layered Materials (CCDM) is one of 10 new Energy Frontier Research Centers founded by the U.S. Department of Energy through a four-year award starting from August 2014. The center, led by Dr. John Perdew develops, applies and validates theoretical methods to calculate the electronic structure of materials. While these methods can be useful for the design of many materials, CCDM focuses on the layered and two-dimensional materials that have potential for clean-energy technologies. CCDM researchers aim to predict how the properties of these materials are affected by composition, structure, interfacial support, defects and strain, and to assist the design of new materials for practical applications. In particular, CCDM seeks to understand catalysis on layered and two-dimensional materials.

Validation and motivation are via experimental synthesis and characterization. The center includes 19 senior investigators from Drexel University, Duke University, North Carolina State University, Northeastern University, University of Pennsylvania, Princeton University, Rice University, University of Texas, and BNL. In addition, the J. Nehru Center for Advanced Scientific Research in Bangalore, India is a collaborator. The annual meeting offers opportunities for all CCDM members to discuss their research and foster new ideas and synergy across the center.

The annual meeting is supported by CCDM, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science. More information available at *http://efrc.cst.temple.edu/*

COLLEGE OF SCIENCE AND TECHNOLOGY

CENTER FOR THE COMPUTATIONAL DESIGN OF FUNCTIONAL LAYERED MATERIALS

2016 ANNUAL MEETING

May 12-13
Science Education and Research Center

TEMPLE UNIVERSITY

College of Science and Technology

All events in Room 110A unless otherwise noted.

MAY 12

8:00-8:30
Breakfast and Registration, Lobby

8:30-8:40
John Perdew Opening Remarks

8:40-9:00
Gus Scuseria, Thrust I leader
Goals, achievements, and future plans of Thrust I: Theory

9:00-9:10
John Perdew
SCAN: An accurate new density functional for the Material Genome Initiative

9:10-9:20
Du Zhang
Excitation energies and ionization potentials from the particle-particle random phase approximation

9:20-9:30
Alejandro Garza
Robust electronic structure methods based on coupled cluster and density functional theories

9:30-9:50
Mikko Haataja
Overview of multiscale modeling of layered materials: Past, present, and future

9:50-10:00
David Srolovitz, Thrust II leader
2H/1T edges and interfaces in MoS_2

10:00-10:10
Arun Bansil
Topological phases harbored in thin film materials

10:10-10:30
Eric Borguet, Thrust III leader
Overview of progress in synthesis and characterization of 2D materials

10:30-10:40
Ian McKendry
Synthetic strategies for enhancing properties of 2D materials

10:40-10:50
Qiao Qiao
Interplay between electronic and structural modulations in quasi-2D materials

10:50-11:10
Coffee break, SERC Lobby

11:10-11:30
Arun Bansil, Forum A leader
Overview of cross-cutting activities of Forum A

11:30-11:40
Maria Iavarone
STM characterization of MoS2 films

11:40-11:50
Liping Yu
Bending effects on the electronic structure of nanoribbons

11:50-12:10
Daniel Strongin, Forum B leader
Making a layered material more catalytically active by computational design

12:10-12:20
Rick Remsing
Frustration leads to success

12:20-12:30
Mike Zdilla
Combining theory and experiment to identify and accentuate key features in water oxidation catalysis

12:30-13:30
Group lunch, SERC Lobby

EAB members and Provost Hai-Lung Dai meet for a private lunch
Room 704

13:30-14:10
Breakout by Thrusts
Thrust I, Room 720
Thrust II, Room 108A
Thrust III, Room 108B

Goran Karapetrov
Competing correlated electrons states in TiSe2

14:15-15:15
Round Table Forum A

Jeb Bates
Guiding experiment with theory; reflecting on the impact of SCAN from molecules to layered materials

Bernardo Barbiellini
Designing bifunctional catalysts for oxygen reduction and evolution

15:15 – 15:30
Coffee Break, SERC Lobby

15:30-16:30
Round Table Forum B

Linyou Cao
Towards extreme manipulation of the chemistry and physics in 2D materials

Akila Thenuwara
Metal confinement in layered oxides: An effective strategy for enhanced water oxidation

Haowei Peng
Planning of high-throughput calculation on 2D materials

16:30-17:15
Executive Committee Meeting
Room 108A

16:30-18:00
Poster Session, SERC Mezzanine

18:30-20:30
Dinner: Sang Kee Peking Duck House
238 N. 9th St, Philadelphia

18:30-20:30
Executive Committee and Advisory Board discussion
Le Chéri, 251 S. 18th Street, Philadelphia

MAY 13

8:30-9:00
Breakfast, SERC Lobby

9:00-10:00
Executive Committee and Advisory Board Members Meeting
Room 720

10:00-10:10
Haowei Peng
SCAN with a long-range vdW correction

10:10-10:20
Shuyang Dai
A multiscale model for the structure of twisted bilayer graphene

10:20-10:30
Xifan Wu
Stabilization of highly polar BiFeO3-like structure: A new interface design route for enhanced ferroelectricity in artificial perovskite superlattices

10:30-10:40
Joel Berry
Stretching, bending, and crystal structure transformations in 2D TMDs

10:40-10:50
Yimei Zhu
Direct observations of photoexcitation induced dynamics of charge density wave and charge-orbital ordered states using ultrafast electrons

10:50-11:00
Xiaoxing XI
Building 2D oxides one atomic layer at a time

11:00-11:10
Yaroslav Aulin
Steady state and ultrafast optical characterization of 2D materials to improve catalysis

11:10-11:20
Dan Trainer
Growth and characterization of MoS2 films

11:30-12:15
Qimin Yan
First-principles data-driven discovery of transition metal oxides for artificial photosynthesis

12:15-12:30
John Perdew closing remarks

12:30 – 13:30
Lunch, SERC Lobby