About the Workshop

One of the holy grails of materials science is the in silico design of novel materials with prescribed properties. Such a capability would allow us to tune material parameters in a way that would reveal up-to-now unrealized behavior. This would also enable a more principled way of developing novel devices and technologies. At the moment this direction of research is rather "aspirational." While "materials design" is a term that appears with increasing frequency in many of the current discussions about the future of materials science, the meaning of the term covers a broad range of unrelated areas and techniques.

The notion that connects these disparate efforts is that with the increasing sophistication of high performance computation, both hardware and software, the complex problem of building a first-principles understanding of materials will eventually be possible. The key intellectual challenge we wish to discuss is to identify tools that explain a sufficiently broad range of the rich spectrum of behaviors observed in complex materials to provide the impetus for moving the field beyond "explanation" to "prediction", a much harder task. Ultimately, this approach goes directly to the heart of emergent phenomena: to what extent can we, with our advanced computational tools and our experience with known emergent phenomena, predict new materials' properties? Discussing this among a group of the world's leading researchers in the field is the goal of this workshop.

Organizing Committee

David Bishop | Boston University
David Campbell | Boston University
Gabi Kotliar | Rutgers University
Andrei Ruckenstein | Boston University
Meigan Aronson | SUNY Stonybrook
Hideo Hosono | Tokyo Insitute of Technology
Karen Hallberg | Centro Atómico Bariloche
Francisco de la Cruz | Centro Atómico Bariloche

Program

FRIDAY, SEPTEMBER 27

8:00 a.m. – 9:00 a.m.	**Breakfast & Registration**
9:00 a.m. – 9:10 a.m.	**Welcome** David Bishop, Boston University
9:10 a.m. – 10:00 a.m.	**Introductory Overview** Gabriel Kotliar, Rutgers University
10:15 a.m. – 1:00 p.m.	**Session I: Solid State Chemistry** Discussion leader: David Coker, Boston University *Evgeny Antipov, Lomonosov Moscow State University* *Hideo Hosono, Tokyo Institute of Technology* *Ni Ni, UCLA* *Hidenori Takagi, RIKEN*
1:00 p.m. – 2:00 p.m.	**Lunch**
2:00 p.m. – 5:00 p.m.	**Session II: The Search for Materials** Discussion leader: Malcolm Beasley, Stanford University *Meigan Aronson, Stony Brook University* *Zachary Fisk, UC Irvine* *Pascoal Pagliuso, UNICAMP* *Darrell Schlom, Cornell University*

Unless otherwise noted, all events will be held in room 906 of the Boston University Photonics Center.

SATURDAY, SEPTEMBER 28

8:00 a.m. – 9:00 a.m. **Breakfast**

9:00 a.m. – 9:45 a.m. **Introductory Overview**
Brian Sales, Oak Ridge National Laboratory

10:00 a.m – 1:00 p.m. **Session III: State of the Art of Theory**
Discussion leader: Karen Hallberg, Centro Atómico Bariloche

Ryotaro Arita, University of Tokyo

Kristjan Haule, Rutgers University

Andrew Millis, Columbia University

Mark van Schilfgaarde, King's College London

Cedric Weber, King's College London

1:00 p.m. – 2:00 p.m. **Lunch**

2:00 p.m. – 5:00 p.m. **Session IV: Tailoring Materials Using Mottness & Hundness**

Discussion leader: Gabriel Kotliar, Rutgers University

Dimitri Basov, UC San Diego

Antoine Georges, École Polytechnique

Marcelo Rozenberg, CNRS

Yasutomo Uemura, Columbia University

6:30 p.m. – 8:30 p.m. **Dinner Reception** at the **Boston University Castle**
225 Bay State Road

SUNDAY, SEPTEMBER 29

8:00 a.m. – 9:00 a.m. **Breakfast**

9:00 a.m – 11:30 a.m **Session V: Novel Materials**
Discussion leader: David Campbell, Boston University

Massimo Capone, CNR-IOM

Kenneth Burch, Boston College

Matthew Rosseinsky, University of Liverpool

11:30 a.m. – 12:30 p.m. **Rapporteur**
Andrei Ruckenstein, Boston University

12:30 p.m. **Lunch, Depart**

Acknowledgements

The organizers would like to thank our sponsors:
ICAM-I2CAM: The Institute for Complex Adaptive Matter
U.S. National Science Foundation
Boston University
The Division of Materials Science and Engineering

One of us, DKC, acknowledge the support of the U.S. National Science Foundation I2CAM International Materials Institute Award, Grant DMR-0844115.

Workshop Staff

Ruth Mason | Director, Engineering Divisions
Daniel Singer | Administrative Assistant, Designer

BOSTON UNIVERSITY