

# COMPUTATIONAL MATERIALS: CHALLENGES & OPPORTUNITIES

PARIS, May 31<sup>st</sup> – June 2<sup>nd</sup>, 2017

<http://paris-meeting-2017.uchicago.edu/>

## Wednesday, May 31<sup>st</sup>

**9:00 – 9:10 Welcome: Robert Morrissey** (Director of UoC Paris Center)

**9:10 – 9:20 Brief introduction to the meeting: Giulia Galli**

**9:20 – 3:30 p.m. Presentation of centers and projects**

*Goals of this session include informing participants of the major activities in each center/project, including software, validation, data-workflows, databases and major applications*

- The ETSF - Lucia Reining (<http://etsf.polytechnique.fr/>)
- Center for computational quantum physics - Antoine George (<https://www.simonsfoundation.org/flatiron-institute/center-for-computational-quantum-physics/>)
- European Materials Modelling Council (EMMC) —Erich Wimmer (<http://emmc.info>; <http://www.materialsdesign.com/about/erich-wimmer>)
- Center for Predictive Simulation of Functional Materials (CPSFM) - Paul Kent (<http://cpsfm.ornl.gov/>)
- Center for Computational Study of Excited-State Phenomena in Energy Materials (C2SEPEM) - Steve Louie (<http://c2sepem.lbl.gov/>)
- MICCoM - Giulia Galli (<http://miccom-center.org/>)
- NOMAD – Claudia Draxl (<https://nomad-coe.eu/>)
- MaX - Elisa Molinari (<http://www.max-centre.eu/>)
- E-CAM - Emilio Artacho (<https://www.e-cam2020.eu/>)
- CECAM—Ignacio Pagonabarraga (<https://www.cecarn.org/>)
- MARVEL - Nicola Marzari (<http://nccr-marvel.ch/>)
- CMI<sup>2</sup> - Shinji Tsuneyuki (<http://www.nims.go.jp/eng/research/MII-I/>)
- The Materials Project - Kristin Persson (<https://www.materialsproject.org/>)
- Open Quantum Materials Database - Chris Wolverton (<http://oqmd.org/>)
- Automatic Flow for materials discovery - Stefano Curtarolo (<http://aflowlib.org/>)
- Suncat - Thomas Bligaard (<http://suncat.stanford.edu/theory>)

**4:00-5:00 p.m. Panel (1) Metadata & Data**—Chair: **Claudia Draxl**: summary on metadata and databases followed by discussion on possible collaborations

## Thursday June 1<sup>st</sup> morning (coffee break at 10:30 a.m.)

**Chair: Lucia Reining**

*Goals include: Understanding how to avoid duplication of efforts and how to leverage complementary efforts; for example: discuss possible collaborations, between centers focused on high-throughput calculations and those focused on method developments; collaborations about definition of metadata, interfaces between databases*

**Panel (2) Software**—Chair: **Xavier Gonze**: summary of software development followed by discussion on possible collaborations; future of open source

**Panel (3) Software versus hardware** funding—Chair: **Jack Deslippe**

**Panel (4) Workflows**—Chair: **Kristin Persson**: summary on workflows followed by discussion on possible collaborations

## Thursday June 1<sup>st</sup> afternoon (coffee break at ~ 3:00 p.m.)

**Chair : Paul Kent**

**Panel (5)** What's the next big thing? How to influence funding agencies in the direction of the next big thing (topics & strategies)? — How to better connect to experimental efforts? Chair: **Nicola Marzari**

**Panel (6)** Sustainability of efforts: education of workforce; dissemination of our work; which publication venues? Chair: **Emilio Artacho**

**8:00 p.m. Dinner at Restaurant de l'Opera**

## Friday June 2<sup>nd</sup>, morning

**Chair: Giulia Galli**

**Discussion of draft document (manifesto)**