AGENDA

Location: Argonne National Laboratory, Building 240, Room 1501

9:00 am - 9:30 am  Introduction to MICCoM-3: goals and expectations—Giulia Galli

Chairs and Discussion Facilitators: Jon Whitmer and Giulia Galli

9:30 am - 10:00 am  State of the SSAGES/PySAGES project – Jonathan K. Whitmer

(20 min + 10 discussion)

10:00 am – 10:30 am  Future Developments in PySAGES – Juan de Pablo

(20 min + 10 discussion)

10:30 am – 11:00 am  Permutationally invariant CV discovery and Biased Sampling -Andy Ferguson.

(20 min + 10 discussion)

11:00 a.m. -11:15 a.m.  Coffee Break

11:15 am – 11:45 am  Integration of Simulation and Machine Learning in Autonomous Materials Discovery – Jie Xu

(20 min + 10 discussion)

11:45 am – 12:15 pm  ML for electronic structure and experimentally-informed sampling– Maria Chan

(20 min + 10 discussion)

12:15 pm – 1:00 pm  Working Lunch

Chairs and Discussion Facilitators: Jon Whitmer and Giulia Galli

1:00 pm – 1:30 pm  Target systems for verification and validation for PySages & ML- Jonathan K. Whitmer (with input from all)

Chairs and Discussion Facilitators: Marco Govoni and Giulia Galli

1:30 pm – 2:00 pm  Status of QDET (Marco Govoni) and Planned Developments (Siyuan Chen)

(20 min + 10 discussion)
2:00 p.m. – 2:30 p.m.  **Status of TDDFT calculations and Planned Developments** (Yu Jin & Shreya Verma)  
*(20 min + 10 discussion)*

2:30 p.m. – 3:00 p.m.  **Planned use of HPC** (Victor Yu) and of hybrid classical-quantum architectures (Benchen Huang)  
*(20 min + 10 discussion)*

3:00 p.m. – 3:15 p.m.  **Coffee Break**

3:15 pm – 3:45 pm  **Target systems for verification and validation for excited states** – Joe Heremans & Marco Govoni *(with input from all)*

3:45 p.m. – 4:15 p.m.  **Status of FPMD (Qbox) and planned developments** – Francois Gygi  
*(20 min + 10 discussion)*

4:15 p.m. – 4:55 p.m.  **Discussion on coupling of sampling and FPMD** (Francois Gygi, Jon Whitmer and Andy Ferguson) *(20 min)* & **Discussion on coupling of sampling and excited states calcs.** (Whitmer & Govoni) (Giulia Galli, Marco Govoni, and Johathan K. Whitmer) *(20 min)*

5:00 p.m. Adjourn