



Midwest Integrated Center  
for Computational Materials

All-Hands MEETING October 31, 2023

## 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 Facilitator:** Giulia Galli

1:30 pm – 1:50 pm **Status of WEST (Marco Govoni) & HPC developments** (Victor Yu)  
*(15 min + 5 discussion)*

1:50 p.m. – 2:20 p.m. **Status of TDDFT calculations and Planned Developments** (Yu Jin & Shreya Verma) *(20 min + 10 discussion)*

2:20 p.m. – 2:50 p.m. **Status of QDET** (Marco Govoni) **and Planned Developments** (Siyuan Chen)

2:50 p.m. – 3:00 p.m. **Status of Quantum Computing & Planned Developments** (Benchen Huang)

*(5 min + 5 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