

2023 Systematic Analysis of Errors and Uncertainty from Materials Modeling & Discovery to Manufacturing: Towards Best Practices Across Scales

Drs. Elif Ertekin (UIUC), Giulia Galli (U. Chicago), and Ali Sayir (AFOSR) |
June 8-9, 2023 | Arlington, VA

Basic Research Innovation Collaboration Center (BRICC)
4100 N Fairfax Drive, Suite 450 | Arlington, VA 22203

Agenda Day 1 | June 8, 2023

Session	Time	Activity
Check-in	8:00-8:30	Registration and check-in
Overview of workshop goals and objectives	8:30-8:45	Welcome – Elif Ertekin, Giulia Galli Opening Remarks – Alexis Lewis (NSF), Ali Sayir (AFOSR)
I. Error control for electronic structure and first principles	8:45-9:05	Nicola Marzari (EPFL)– Uncertainty/error control in density functional theory
	9:05-9:45	Emanuel Gull (Michigan), Lucas Wagner (Illinois) - High-accuracy:Simons Collaboration lessons learned from benchmarking experiences
	9:45-10:05	Geoffroy Hautier (Dartmouth) – Uncertainty/error control in applying first principles simulations in high-throughput mode
	10:05-11:05	Group Discussion – Karsten Jacobesen (DTU), Wennie Wang (UT Austin)
II. Error Control in the application of ML/AI/data science to materials	11:05-11:25	Joshua Schrier (Fordham) – Integration of physics-based models and machine learning, autonomous AI-driven materials design
	11:25-11:45	Boris Kozinsky (Harvard) Active learning MD potentials:NEquip;on-the-fly corrections
	11:45-12:05	Roberto Car (Princeton) – DeepMD Neural Networks for solvation, chemical reactions.
	12:05-1:20	Group Discussion over Working Lunch – Rafael Bombarelli (MIT), Andrew Gordon Wilson (NYU)
III. Best practices for modelers when working with experimentalists	1:20-1:40	Annabella Selloni (Princeton) – Oxide surfaces, water, connecting simulations to experiments
	1:40-2:00	Michelle Johannes (NRL) – Benchmarking for correlated materials and oxides, connecting simulations to experiments
	2:00-2:20	Sage Bauers (NREL) – Integration High throughput experimentation with first principles; perspectives from experiment
	2:20-3:20	Group Discussion – Wolfgang Windl (Ohio State), Vladan Stevanovic (Colorado School of Mines)
Poster Session	3:20-5:00	Participant posters
5:00	Adjourn	

2023 Systematic Analysis of Errors and Uncertainty from Materials Modeling & Discovery to Manufacturing: Towards Best Practices Across Scales

Drs. Elif Ertekin (UIUC), Giulia Galli (U. Chicago), and Ali Sayir (AFOSR) |
June 8-9, 2023 | Arlington, VA

Basic Research Innovation Collaboration Center (BRICC)
4100 N Fairfax Drive, Suite 450 | Arlington, VA 22203

Agenda Day 2 | June 9, 2023

Session	Time	Activity
Check-in	8:30-8:50	Registration and check-in
Reconvene	8:50-9:00	Recap/Review – Ertekin, Galli, Sayir
IV. Error control for materials synthesis, processing, and manufacture	9:00-9:20	Raymundo Arroyave (Texas A&M) – materials modeling across length scales, microstructure evolution, and design/optimization under uncertainty
	9:20-9:40	Chenhui Shao (Illinois) – Uncertainty prediction of process modeling
	9:40-10:00	Jason Hattrick-Simpers (U. Toronto) – automated experimental platform & AI control over composition, processing for high performance/industrial materials
	10:00-11:00	Group Discussion – Lili Cai (Illinois), Ale Strachan (Purdue)
V. Incorporating error analysis into workflows and materials data repositories	11:00-11:20	Jane Greenberg (Drexel)- metadata errors/challenges, data workflows, RCR – reproducible computational workflows, FAIR
	11:20-11:40	Stefano Curtarolo (Duke) – need & opportunities for uncertainty/error analysis in online first-principles databases and repositories like AFLOW
	11:40-12:00	Daniel Wines (NIST) – need & opportunities for incorporating error/uncertainty into platforms for automated materials discovery/optimization like JARVIS
	12:00-12:20	Mark Transtrum (BYU) – UQ tools for practitioners based on information geometry, OpenKIM
	12:20-1:30	Group Discussion and Working Lunch – Sterling Baird (Utah), Elif Ertekin (Illinois)
Closing	1:30-2:00	Closing discussion, next steps
2:00	Adjourn	