

第4回講演会のお知らせ

Connecting Theory and Experiment for Closed-Loop Materials R&D

Faster materials discovery depends increasingly on combining physics-based modeling, machine learning and experimental measurements in one consistent data ecosystem. This presentation discusses a data-centric approach to materials R&D. In it, physics-based methods such as density functional theory and molecular dynamics, along with machine-learning models, connect to experimental data streams through shared FAIR, JSON-based data standards and repeatable workflows. I will first outline the architecture of such a platform. I will then show use cases where automated high-throughput simulations and interoperable data formats speed up property prediction for heterogeneous interfaces and semiconductor-relevant materials. This builds on prior work on data-centric online ecosystems and model ontologies for computational materials science. Next, I will describe recent theory-experiment case studies with academic and national laboratory partners, which show how simulations and laboratory data can refine each other in a closed loop. Finally, I will discuss open-source data conventions and tools for categorizing models and workflows, and how these standards can work with experimental data infrastructure being built at laboratories in the USA and Japan to support reproducible multiscale simulations for future semiconductor and quantum materials devices to help achieve scientific superintelligence.

[1] Bazhiron, arXiv:1902.10838 (2019);

[2] Zech & Bazhiron, J. Chem. Inf. Model. 62, 1268 (2022);

[3] Kalinin & Bazhiron et al., Microscopy & Microanalysis. 32, 1 (2026)

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16:00-17:30

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講師

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Timur Bazhiron, Ph.D.

Brief professional Biography: Timur Bazhiron, Ph.D. (USA native), CEO/Founder of Exabyte Inc. (the developer of Mat3ra.com). Timur holds a Ph.D. in Physics from the University of California at Berkeley and has been the CEO of Exabyte Inc. since its inception in 2014 pioneering the field of Materials Informatics / AI for Materials R&D. Mat3ra.com (the product of Exabyte Inc.) is a cloud-based platform enabling materials scientists in energy, semiconductor, and manufacturing, to rapidly adopt and deploy a wide variety of digital techniques to develop new materials faster. The company is funded by Tim Draper, the Peter Thiel foundation, as well as US Air Force Ventures. Mat3ra has dozens of Global 2000 customers, including ENEOS and Merck KGaA, , works with multiple US-based governmental institutions, including multiple US DoE laboratories, NRL, AFRL, NIST, and allows 45,000+ scientists worldwide to collaborate and generate quality intelligence accelerating the pace of materials R&D.

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