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# ACCELERATED MATERIALS AND MOLECULAR DISCOVERY AND OPTIMIZATION WITH AUTONOMOUS FLUIDIC LABS


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ETH Hönggerberg, HCI J 3


Abstract: The current human-dependent nature of experimental research in chemical and materials sciences fails to identify technological solutions for renewable energy, sustainability, and healthcare challenges in a short timeframe. This limitation necessitates the development and implementation of new strategies to accelerate the pace of discovery. Recent advances in reaction miniaturization, robotics, automated experimentation, and artificial intelligence (AI) provide an exciting opportunity to reshape the discovery and manufacturing of new molecules and materials through human-AI-machine collaboration. In this talk, I will present the recent work in my lab on the development of Self-Driving Labs (SDLs) as intelligent robotic co-pilots to human researchers to accelerate discovery, development, and manufacturing of advanced functional materials and molecules by 100×-1000× compared to the status quo. I will discuss how modularization of different chemical synthesis and processing stages in tandem with a constantly evolving machine learning modeling and decision-making under uncertainty can enable a resource-efficient navigation through high dimensional experimental design spaces (>1020 possible experimental conditions). Example applications of SDLs for the autonomous synthesis of colloidal quantum dots and specialty chemicals will be presented to illustrate the potential of autonomous robotic experimentation in reducing synthetic route discovery timeframe from >10 years to a few months. Finally, I will present the unique reconfigurability aspect of SDLs to close the scale gap in chemical and materials research through facile switching from the reaction exploration/exploitation to smart manufacturing mode.


Bio: Milad Abolhasani is an ALCOA Professor and a University Faculty Scholar in the Department of Chemical and Biomolecular Engineering at North Carolina State University. He received his Ph.D. from the University of Toronto in 2014. Prior to joining NC State University, he was an NSERC Postdoctoral Fellow in the Department of Chemical Engineering at MIT (2014-2016). At NC State University, Dr. Abolhasani leads a diverse research group that studies self-driving labs tailored toward accelerated discovery, development, and manufacturing of advanced functional materials and molecules using fluidic micro-processors.

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