CAPeX Pioneer Lectures

Toward Realizing Self-Driving Laboratories: A strategic checklist

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Date and Time	**Location**	Registration by 30 April
Thursday the 2nd May 14:00-15:00, followed by networking to 16:00	Technical University of Denmark, Fysikvej, building 311, meeting room 001, 2800 Kgs. Lyngby	https://forms.office.com/e/q2YKgtJfhc

During the past decade, automated high-throughput research has evolved from “toy problems” to enabling instances of materials development and translation on compressed timelines. Self-driving labs (SDLs) take this a step further, by integrating automated high-throughput experimental (HTE) hardware with computational planning tools (inverse design algorithms, optimization algorithms, and advanced data-management systems). Although the allure of rapid progress pulls interest to SDLs, achieving tangible results requires a strategic coupled investment in both infrastructure and research. This investment necessitates a deliberate, thoughtful approach contrary to the typical rush for immediate outcomes. In other words, to speed up, one must slow down and think.

In my presentation, I’ll introduce a checklist developed over a decadal effort to expedite early-stage R&D. This checklist is based on our experiences in designing custom hardware, integrating both hardware and software into materials-discovery workflows, and customizing machine-learning algorithms specifically for these applications. I will guide the audience through each item on the checklist, providing case studies that highlight both successes and setbacks:

- Selecting tractable problems for “automated” and “autonomous” systems.
- Increasing the odds that materials predicted by generative AI are experimentally accessible.
- Ensuring reproducible, transferable, and “scale-up-able” synthesis.
- Choosing whether to buy or build (home-built automation equipment).
- Performing rapid phase identification to validate synthesis.
- Venturing beyond standard optimization to find novel “exceptional” materials.
- The human side: lessons of leadership, team building, resources, institutional culture, and committing to courageous change.

Tonio Buonassisi (MechE) combines machine learning and high-throughput experiments to create new materials & systems with societally beneficial applications. His early career research in solar energy and techno-economic analysis assisted dozens of companies and earned him a PECASE bestowed by President Obama. In 2018 he served as founding director of the Accelerated Materials Development for Manufacturing (AMDM) programme in Singapore, a S$24.7M effort to accelerate the rate of novel materials development by >10x. He returned to MIT full-time in December 2021, where he leads the Accelerated Materials Laboratory for Sustainability and directs a Department of Energy-funded research center called ADDEPT, in which industry and university partners co-develop more durable perovskite-based tandem photovoltaic (PV) modules using AI/ML and HTE.