# **Self-Driving towards the Best Organic Laser**

Han Hao

Staff Scientist



Acceleration Consortium



# Material Acceleration Organization





# Organic Solid-State

Lasers











## **OLED Market**

- 7.6 Billion Market Cap
- PE Ratio ~40
- Materials/Tech centric business
- Work with external manufacture
- IP heavy
- 28 years in the commercialization

### **OLED Analyst Ratings**

## Strong Buy

Based on 7 analysts offering recommendations for 'OLED' in the last 3 months.

## Analyst Firms Making Recommendations

- B OF A GLBL RES
- CITIGROUP
- COWEN & COMPANY
- DEUTSCHE BK SEC
- NEEDHAM & CO.
- OPPENHEIMER HLD
- ROTH CAPITAL PA

Analyst

\$178.29

Based on **analysts** offering 12 month price targets for **OLED** in the last 3 months. The average price target is **\$178.29** with a high estimate of **\$210** and a low estimate of **\$110**. Sign in to your SmartPortfolio to see more analyst recommendations.



# From OLED to OSLD



- Chihaya Adachi, Kyushu Uni
- Inventor of 3<sup>rd</sup> and 4<sup>th</sup> Gen OLED
- State-of-the-art OSL
- ~10 materials in 3 years



*Adv. Funct. Mater.*, **2018**, *28*, 1802130; *Adv. Optical Mater.* **2020**, *8*, 2000784; *ACS Materials Lett.* **2020**, *2*, 161-167



Solution processable

H13C6 C6H13

Enhanced Stability

# Self-Driving Lab 8 **ACDC Workflow**













Science, **2018**, *361,* 360



## Self-Driving Laboratories (SDLs)





Chem. Rev. 2024, 124, 9633-9732



# **Self-Driving Laboratories (SDLs)**







## "MADNESS" Team



Alán Aspuru-Guzik (Toronto)



Marty Burke (Urbana-Champaign)



Bartosz Grzybowski (Warsaw)



Lee Cronin (Glasgow)



Jason Hein (Vancouver)



# **Function Oriented Molecule Design to Brightest Molecule**





# **Al-Informed Suzuki**

- Good reaction conditions are rare
- Literature mining failed

- General condition optimization
- Four rounds of automated reactions
- 21-46% improvement





# **Deeper Insight into Reaction Progress**

- Time-course tracking with *in-situ* and online monitoring
- Robotic operation and vision control





- Active decision making
- Highly purified material

UNIVERSITY OF TORONTO

ACS Catal. 2020, 10, 13236-13244, Org. Process Res. Dev. 2015, 19, 1809-1819

# **End-to-End Automation Workflow**



- Automated purification and highquality spectroscopic data in ~30 min
- Fast and furious approximation of laser performance in solution













# **Cross-Platform Knowledge Transfer**

- Multiple automated synthesis platforms
- XDL: universal language for chemistry

- Seamless knowledge transfer
- Platform independent reproducibility





*Science* **2019**, *363*, 144, *Science* **2020**, *370*, 101; *Nat. Synth.* **2024**, *3*, 488









500 Candidates

10 molecules in 3 years40 molecules in 1 year500 molecules in 3 months









- Established molecular representation failed
- No obvious structure-property correlations













## **Asynchronous Bayesian Optimization**











# Acceleration Consortium

# Bringing Industry, Government and Academia Together

IENCE

'Self-driving' AI lab awarded \$200M grant to pursue new drugs, materials

By Kathryn Mannie • Global News Posted April 28, 2023 10:53 am · Updated April 28, 2023 11:03 am



Left: The robotic arm with computer vision pours a clear liquid from a beaker into another glass container. Right: A scientist assembles a liquid dispensing tool onto the tool holder of the automated chemistry robot system. James Morley/The Matter Lab/Acceleration Consortium, University of Toronto



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Based at the University of Toronto (UofT), the Acceleration Consortium (AC) is a global community of academia, industry, and government that is accelerating the discovery of new materials and molecules for a sustainable future.





# **Structured For Economic & Social Impact**







## RESEARCH INSTITUTES UNIVERSITY OF TORONTO



## **STAFF SCIENTISTS**

FACULTY

VON

LILIENFELD



SHKURTI

ASPURU-

GUZIK



vision

**ROBOTICS &** 

humanrobot teaming

A CENTRAL AI & AUTOMATION RESEARCH HUB TO

robotic, Al-driven workflows in SDLs 1 – 7





high-throughput

density functional

theory and

physics-

informed

simulations

... and more

solve the research challenges to enable the accelerated, autonomous,

## AI AND LAB ORCHESTRATION





experimental optimization

material representatio



database engineering

language models for science









Feature Importance in the Experimental Design Space









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Canada

NRC CNRC

## **RESEARCH INSTITUTES**

UNIVERSITY OF

TORONTO

#### A MODULAR, AUTONOMOUS, HIGH-THROUGHPUT, SELF-DRIVING LAB FOR

solid-state inorganic materials discovery lab with diverse synthesis, characterization, and application testing modules

## **STAFF SCIENTISTS** MATERIALS alloys, oxides, sulfides, nitrides phosphides, ... SHAYESTEH BAI LI porous materials FACULTY thin-films SINTON HATTRICKnanoparticles and SIMPERS nanostructures MOOSAVI zou

## electrochemical durable, corrosionresistant structural carbon materials conversion green batteries Ю hydrogen production ... and more

**APPLICATIONS** 



carbon capture







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organic small molecule closed loop discovery spanning synthesis, workup, separation, characterization, and application testing











# **Liquid-Liquid Extraction**









Acceleration Consortium

# **Bridging Electronic to Decision Making**





Device, 2024, 100567





Acceleration Consortium Device, 2024, 100567

45





Matter, 2024, 10.1016/j.matt.2024.04.022





# **Do We Need Figure "8"?**









Acceleration Consortium Digit. Discov, 2025, 4, 326-330

48





Digit. Discov, 2025, 4, 326-330

## El Agente, an autonomous Al for performing computational chemistry





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## A MODULAR, AUTONOMOUS, HIGH-THROUGHPUT, SELF-DRIVING LAB FOR

medicinal chemistry with AI assisted close loop design-make-test cycles for developing chemical probes



## **APPLICATIONS**

tools for target validation and safety in cellular and organoid models

starting points for drug discovery



ARROWSMITH

SANTHAKUMAR

BROWN

**FACULTY** 

**RESEARCH INSTITUTES** 

**STAFF SCIENTISTS** 

TORONTO **WUHN** 

BROWN

GREEN

BATEY

# **SDL3 – Drug Discovery**





# **SDL4 – POLYMERS**

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## UNIVERSITY OF TORONTO

## **STAFF SCIENTISTS**



MILLS GUPTA MELVILLE



**FACULTY** 



TRAN SEFEROS

## A MODULAR, AUTONOMOUS, HIGH-THROUGHPUT, SELF-DRIVING LAB FOR

facilitating polymer materials research in urgent but complex applications in health, sustainability and energy



# **APPLICATIONS**



sustainable plastics membranes thin-film electronics batteries

... and more





# **SDL5 – FORMULATIONS**

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formulating materials to address functional needs across personal care, health, and more

## **STAFF SCIENTISTS**





LE DÉVÉDEC ABDOLLAHI CLASKY



BAO





ALLEN

















# 0 0

**APPLICATIONS** 



personal care products

functional food

medicines











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# **SDL6 – HUMAN ORGAN MIMICRY**

of functional tissues and diseases

tissue models with

functional outputs

.00

long-term

culture

tissue/organoid

multifaceted

## **RESEARCH INSTITUTES**



**EXAMPLE HIGH-FIDELITY MODELS** 

... and more

vascularized

d models

tissue/organoi

patient-derived cancer

organoids expansion

and screening

immunocompeten

t tissue/organoid

models

discovery of new materials and therapies using high fidelity models



## **STAFF SCIENTISTS**



















































#### **SDL6 – Human Organ Mimicry** Human Organ Mimicry Self-Driving Lab UNIVERSITY OF 8 ANILIU Brain Cardiac Muscle Breast Cancer Skeletal Muscle Vasculature Liver Monitoring module Aseptic sample preparation module Fat Retrieve Kidney Prepare Store Dispense Shake Move Move Ronaldson-Bouchard et al **Nature Biomed** 2022 Duong et al **Scientific Reports**, 2021 Pierter et al. **Biofabrication**, 2022 Landau and Zhao et al, **Cell Stem Cell**, 2024 from Imaging Heat sample sample reagents stage sample storage Zhao et al Unpublished





## **RESEARCH INSTITUTES**

# UBC

THE UNIVERSITY OF BRITISH COLUMBIA

## **STAFF SCIENTISTS**



LIN

TRUSHINA









BERLINGUETTE HEIN

## A MODULAR, AUTONOMOUS, HIGH-THROUGHPUT, SELF-DRIVING LAB FOR

synthesis and purification scale-up of materials and molecules from SDLs 1-6 with tech and protocol development to bridge commercialization gaps

## organic material synthesis and purification scale-up



chemistry optimization activator, solvent, additive, reagent screening, ...

**EXAMPLE SCALE-UP TASKS** 



process optimization sample prep, visionguided analysis, data sampling and processing







... and more

# SDL7 – Scale Up

## Method development and pre-reaction tasks

IvoryOS

0

- Tech transfer protocols
- HPLC method optimization

## Reaction execution and monitoring

- Automated kinetic studies
- Aut. org synthesis with HPLC monitoring and feedback loops
- Biphasic reaction online monitoring
- ADC synthesis and characterization SDL

## **Workup and purification**

- Automated liquid-liquid extraction
- Robotic Purification
  Optimization Platform
  (solubility screening, cooling crystallization)







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# **INDIGENOUS SCIENCE & ETHICAL SUBSTANCE LAB**

#### **RESEARCH INSTITUTES**



TECHNOSCIENCE RESEARCH UNIT



## **STAFF SCHOLARS**



## FACULTY



MURPHY BOS

## **A RESEARCH HUB TO**

ensure the ethical integration of Indigenous knowledges and values into research design for materials discovery

## **OVERARCHING AIMS**

- To create visions and protocols to ground scientific work in Indigenous and environmental values
- To develop understandings of ethical substance (material, process, governance)
- To co-create research ethics and practices with SDLs

## **APPROACHES**

- Land-based, communitybased, and artsbased approaches grounded in Indigenous Data Sovereignty
- Collaboration • with community researchers

## **GUIDING VALUES**

- Care & reciprocity •
- Timeliness
- Processual consent ٠
- Sustainability and harm • reduction
- Data justice
- Collective benefit, community • governance, and accountability
- Accessibility and open • listening
- Meaningful transformation •

# LAB FOR THE MANAGEMENT OF SCIENCE AND TECHNOLOGY

## **RESEARCH INSTITUTES**



## **STAFF SCHOLAR**



## FACULTY



GOLDFARB

### A RESEARCH HUB DEDICATED TO

advancing our understanding of how scientific discovery and innovation can be managed more effectively. Using the tools of empirical social science, we explore the dynamics of scientific work, with a focus on improving research processes, technology adoption, and the broader systems that enable scientific and technological progress.

#### **OVERARCHING AIMS**

- 1. Al and Automation in Science: We investigate how artificial intelligence and automation are transforming the landscape of scientific discovery, with a focus on their impact on research processes, efficiency, and the future of innovation.
- 2. Barriers to Commercialization: We seek to understand and address the challenges that prevent the effective translation of scientific discoveries into real-world applications
- 3. Policy for Science and Innovation: We work to inform and shape policy that can enhance the productivity of science and innovation systems, ensuring they deliver societal and economic benefits.

# A Home for the AC







# Acknowledgements







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Dr. Felix Strieth-Kalthoff







Acceleration

# Create a materially better future at the 2025 Accelerate Conference in Toronto

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Toronto • Aug 11 — 14, 2025

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Toronto • Aug 11 — 14, 2025

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