

Introduction to the AI-Accelerated Materials Discovery Master Project **Materials for Clean Fuels Challenge Program**

Isaac Tamblyn
Master Project Leader

Challenge Programs



Materials for Clean Fuels



High-throughput and Secure Networks



**Disruptive Technology Solutions for
Cell and Gene Therapy**



Artificial Intelligence for Design

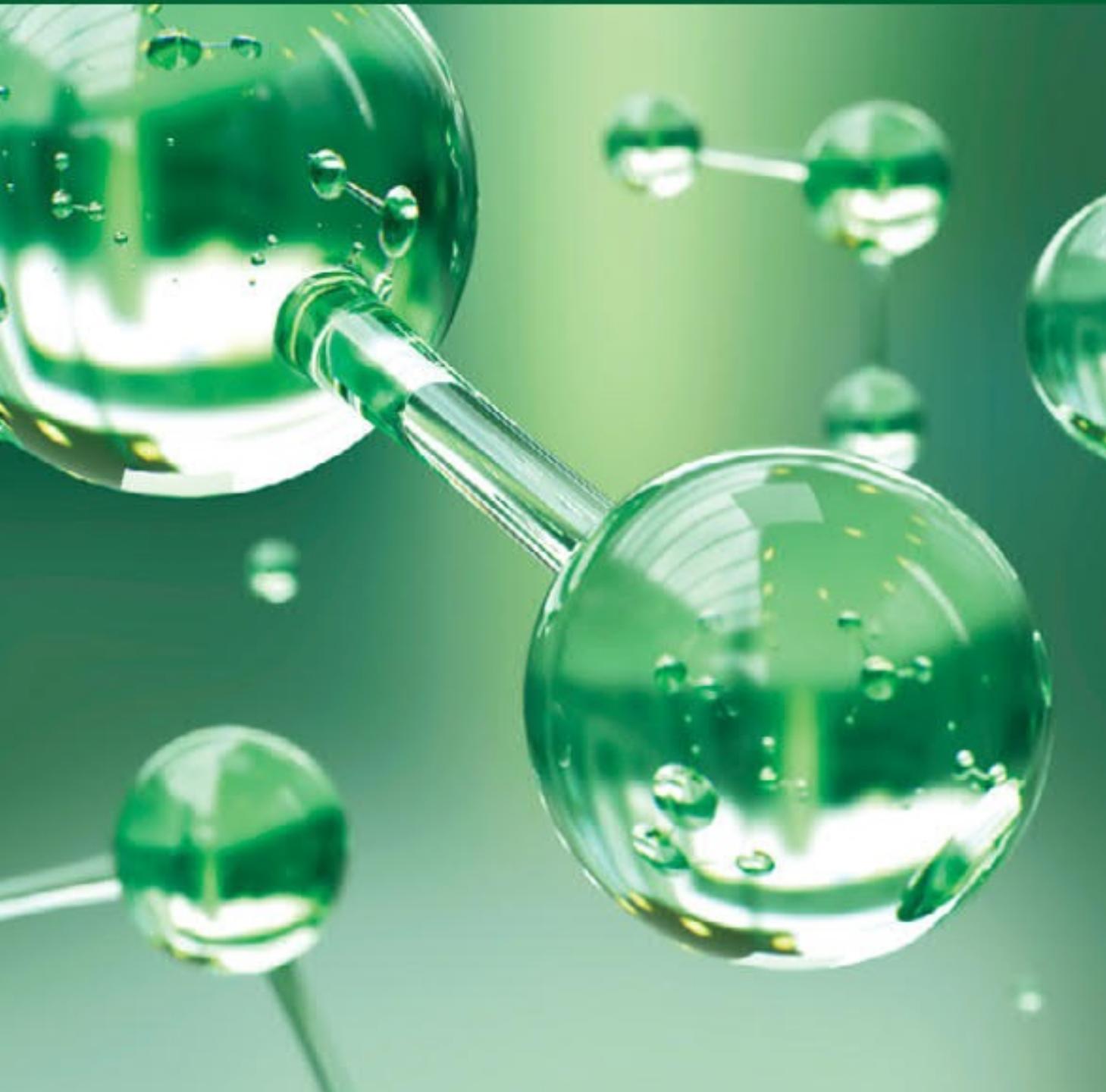
UPCOMING CHALLENGES (2021)

- The North (infrastructure, remote health)
- Quantum Internet of Things
- Aging in Place



MATERIALS FOR CLEAN FUELS

Developing new materials for the production
of renewable fuels and chemical feedstocks



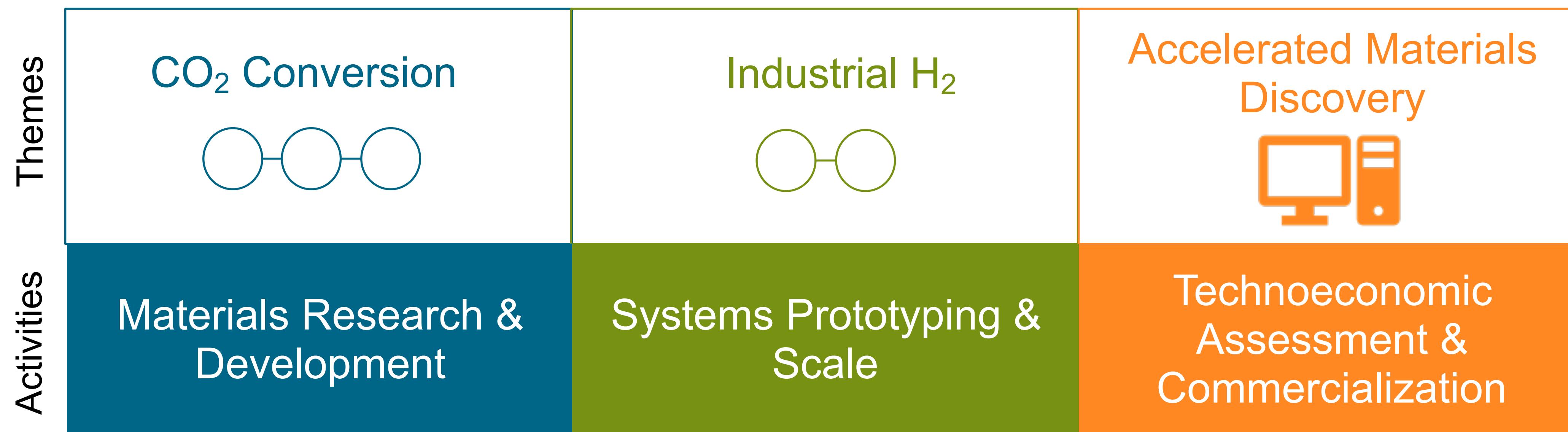
Materials for Clean Fuels

- 7-year \$57M CAD **collaborative** research program
- Collaboration funding available for academics & SMEs
- Transformative high-risk, high-reward technologies at a low technology readiness level (**TRL 1-4**)
- Next-generation materials for CO₂ conversion, H₂ production, and AI for materials discovery



Challenge Program

Goal | Develop innovative materials for renewable fuels & chemical feedstocks



Outcomes | Economically viable processes for CO₂ conversion, H₂ production and future renewable fuels production

Evaluation | Publications, patents, # HQP, cost reduction against incumbents, spinoff companies, # new materials



AI Materials

Accelerated simulation

Generative materials

Augmented measurements

Literature pattern
detection

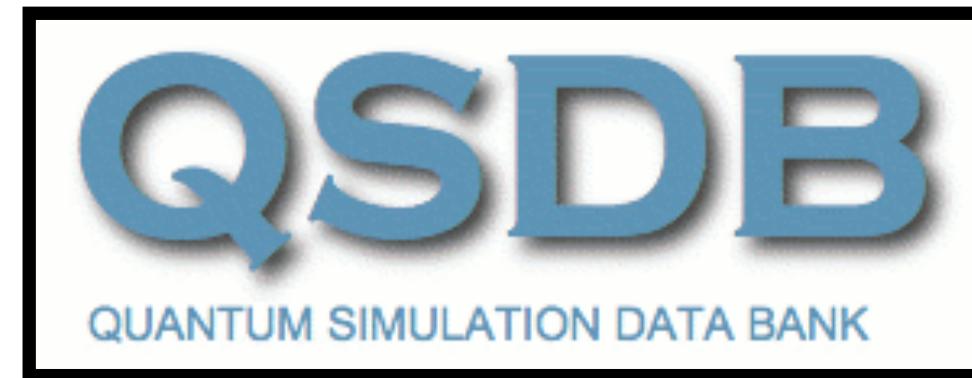
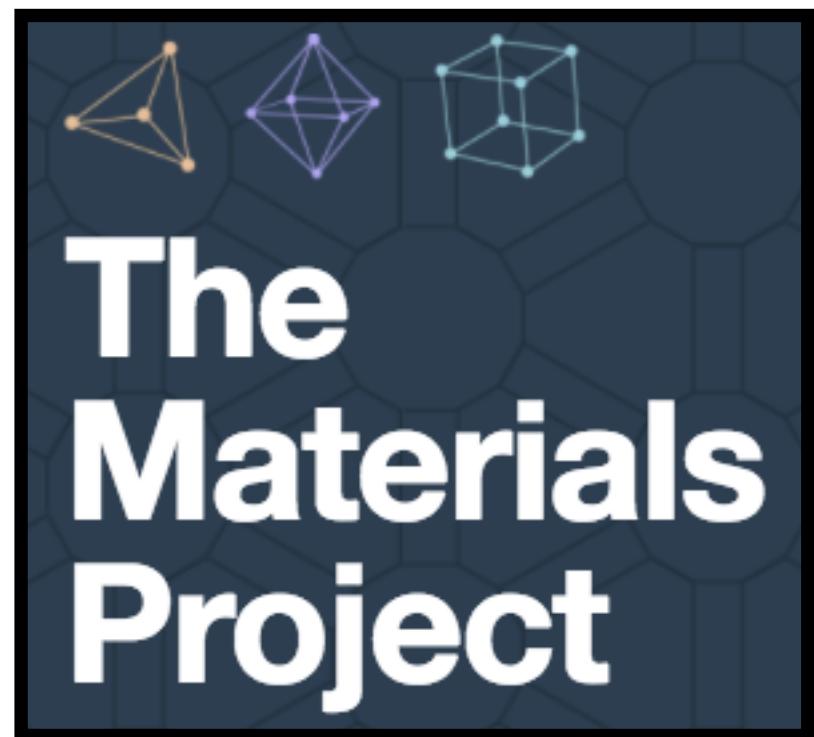
Automated robotic
laboratories

Guided self-assembly

There are a lot of databases

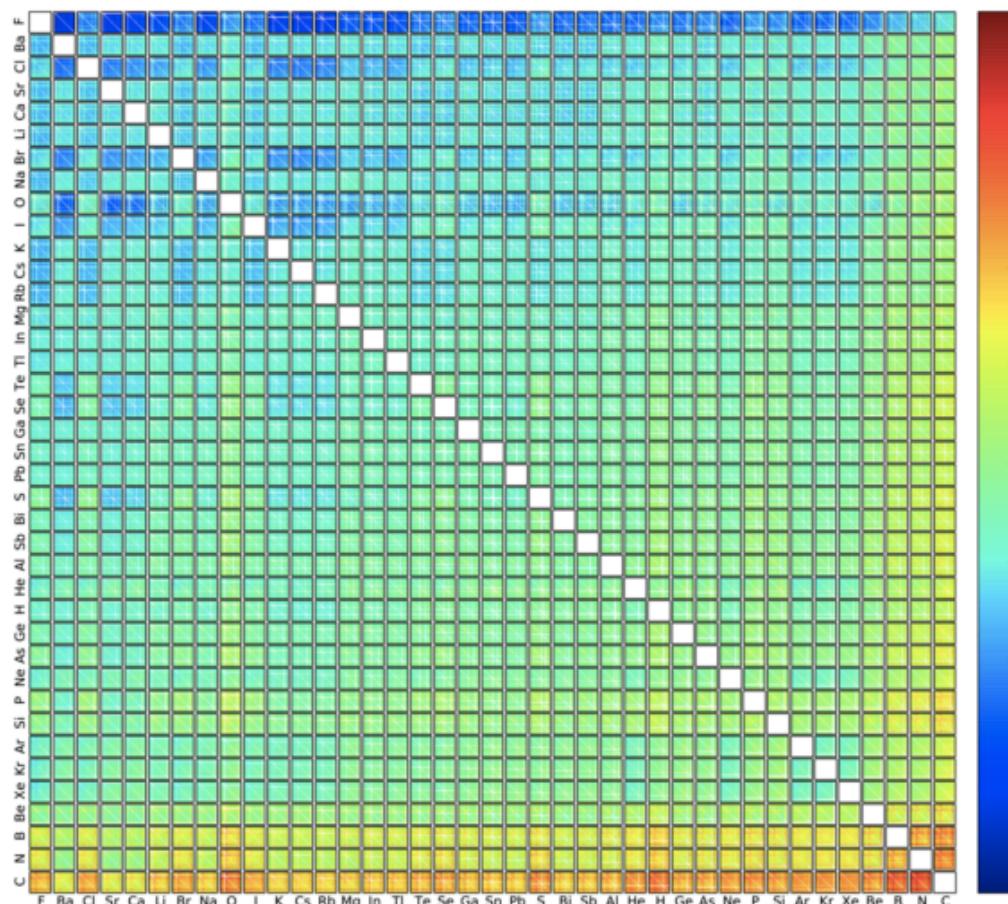
OQMD:

The Open Quantum Materials Database

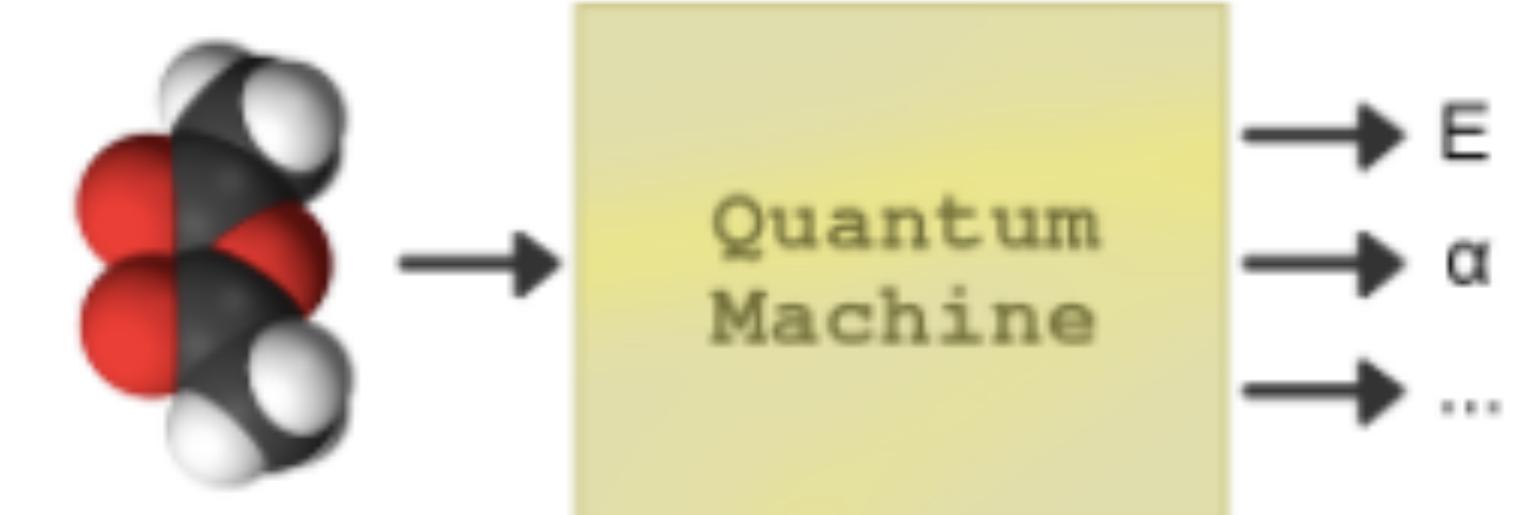


CEPDB – the Harvard
Clean Energy Project Database

◆ MoleculeNet



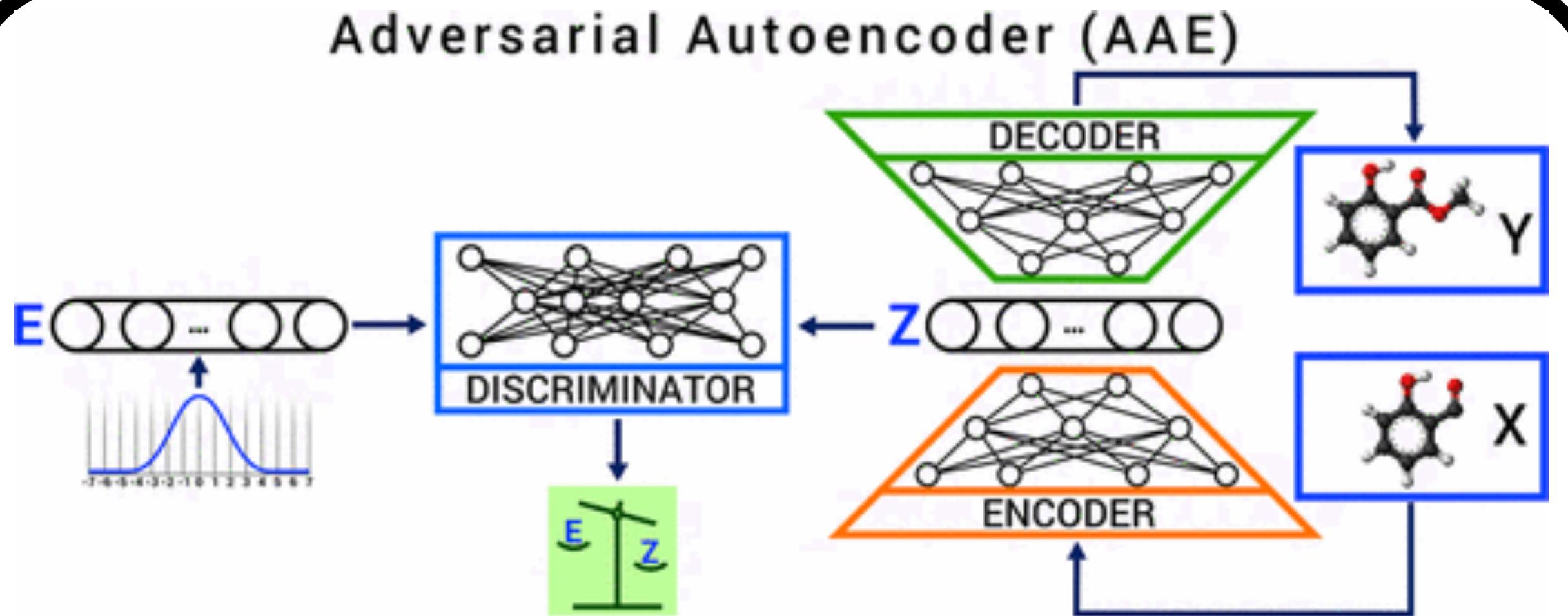
QM7/QM8/QM9... Datasets



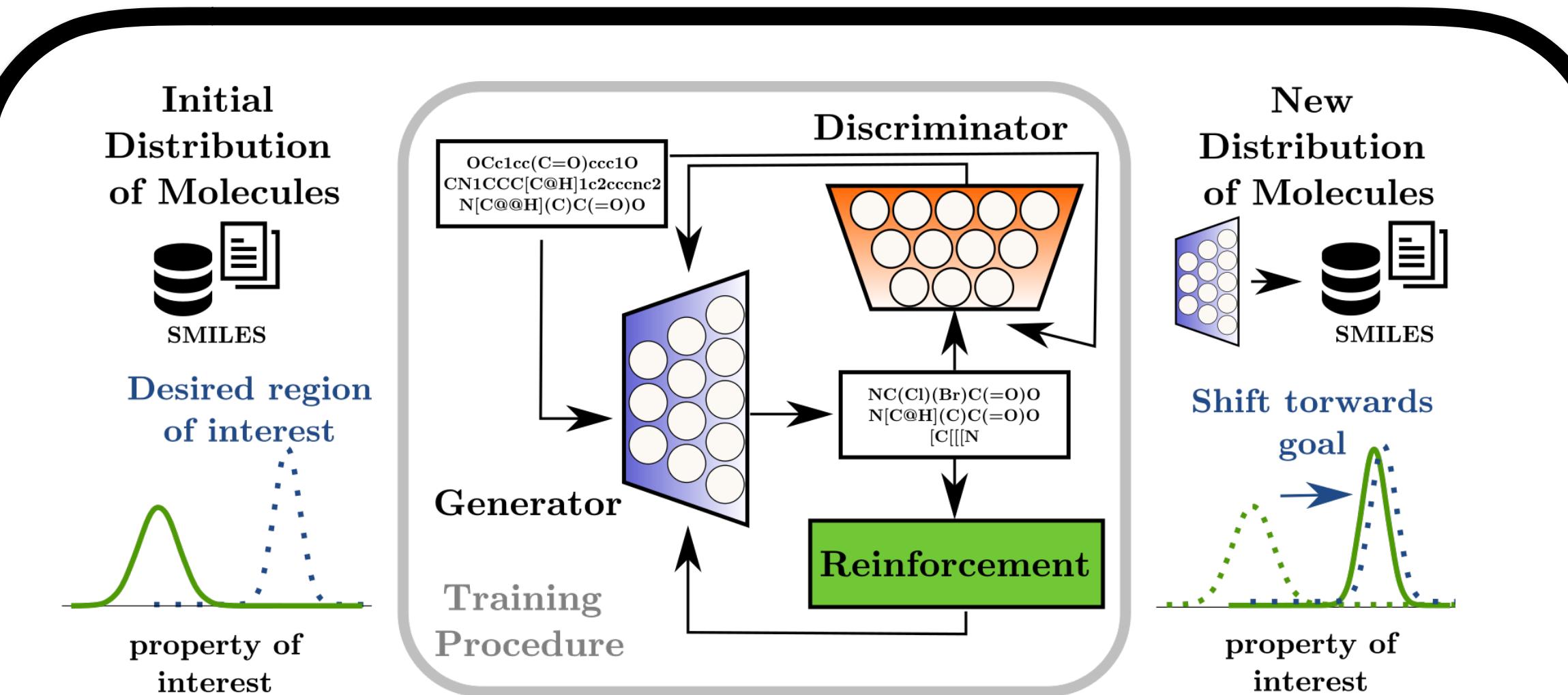
PRL 117, 135502 (2016)

[many others exist]

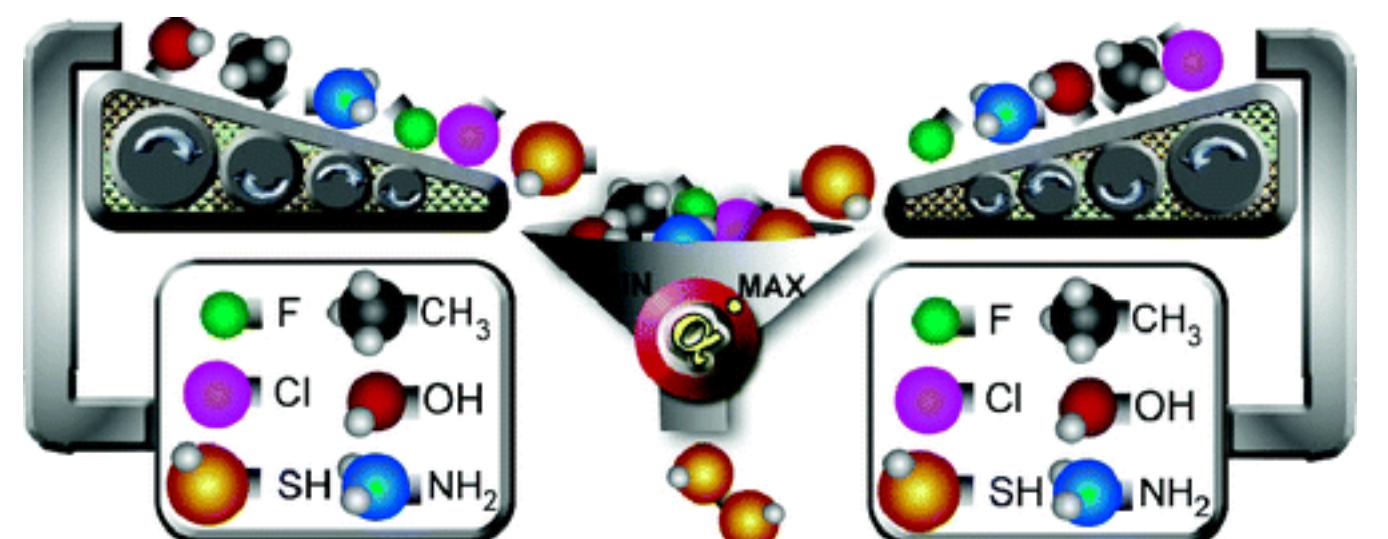
Given some observations...



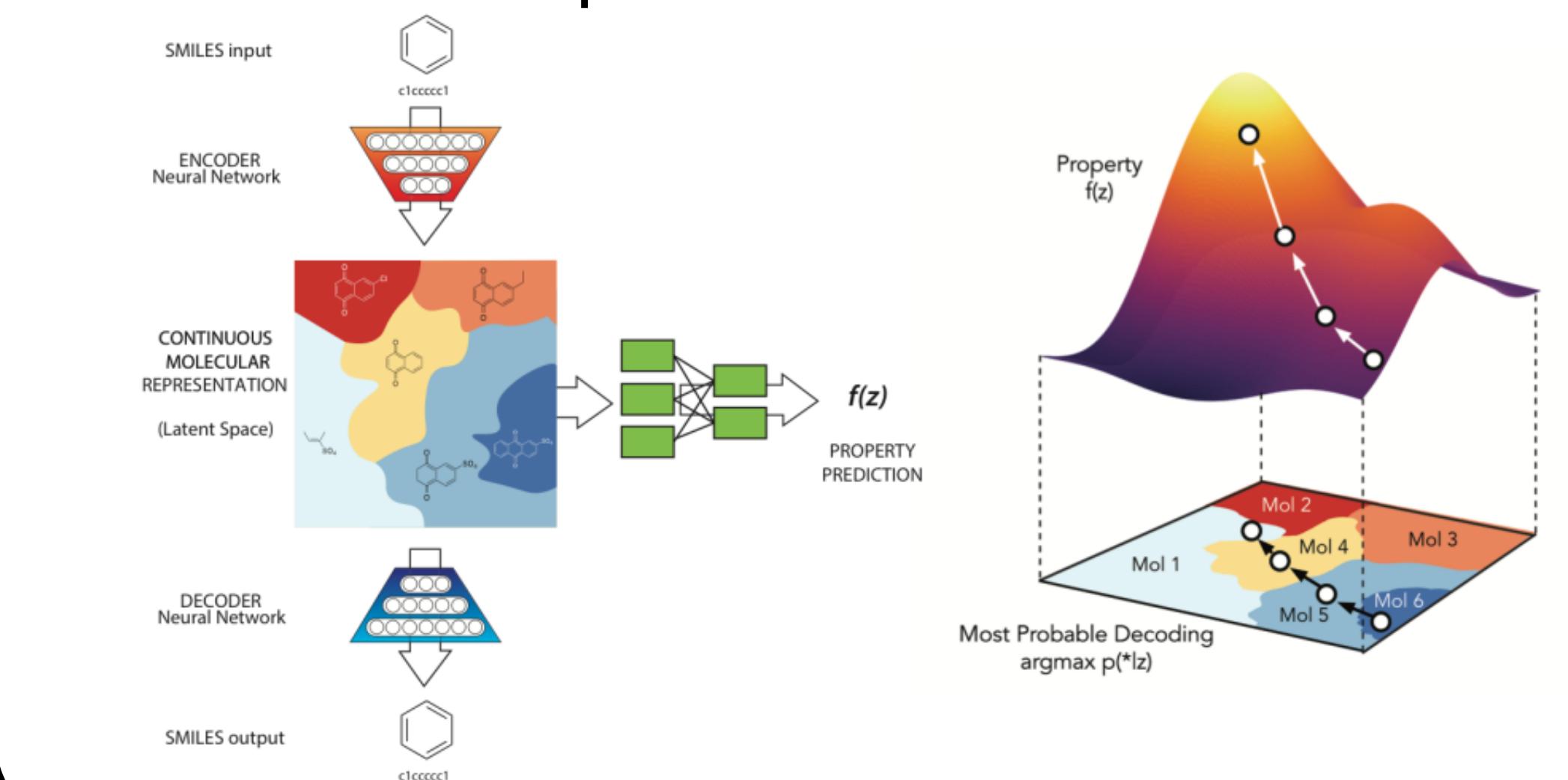
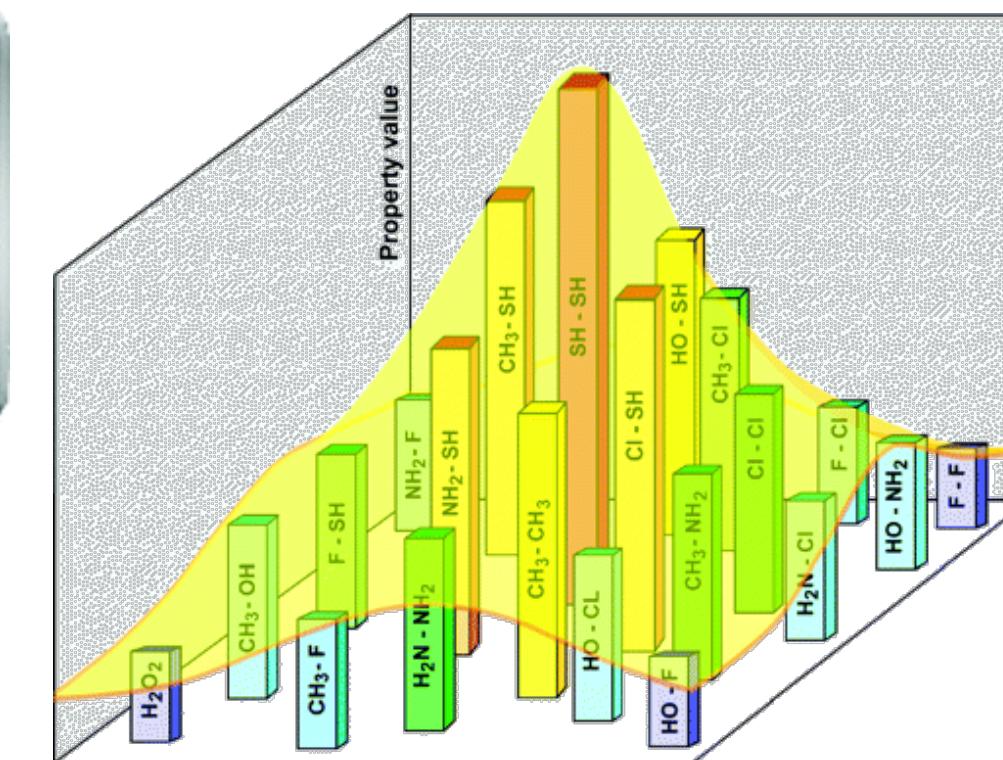
10.1021/acs.molpharmaceut.7b00346



<http://matter.toronto.edu>

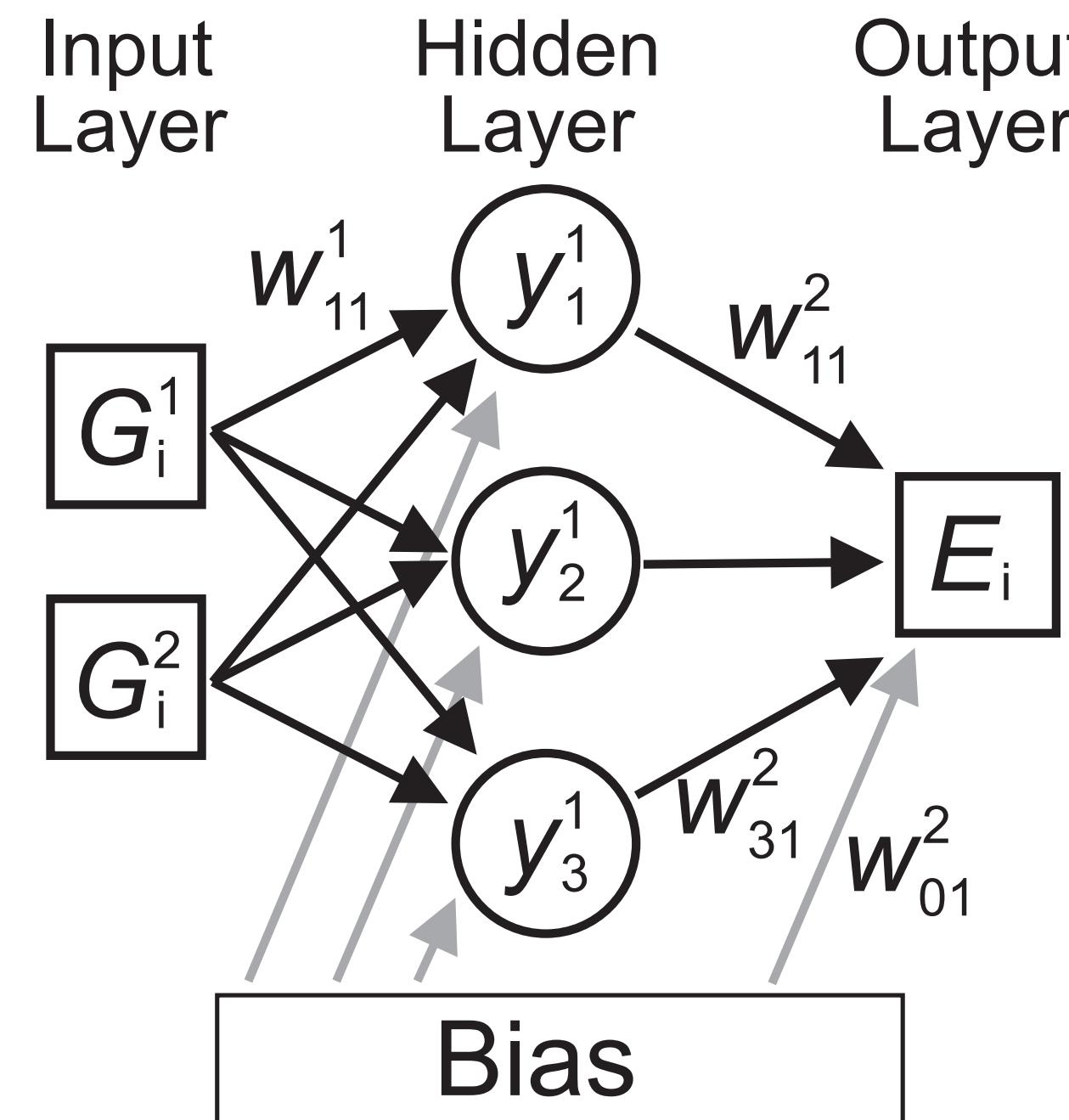


Wang, JACS, 128, 3228, (2006)



Given a structure...

symmetry basis
functions



what are its “properties”?

How shall I describe it?

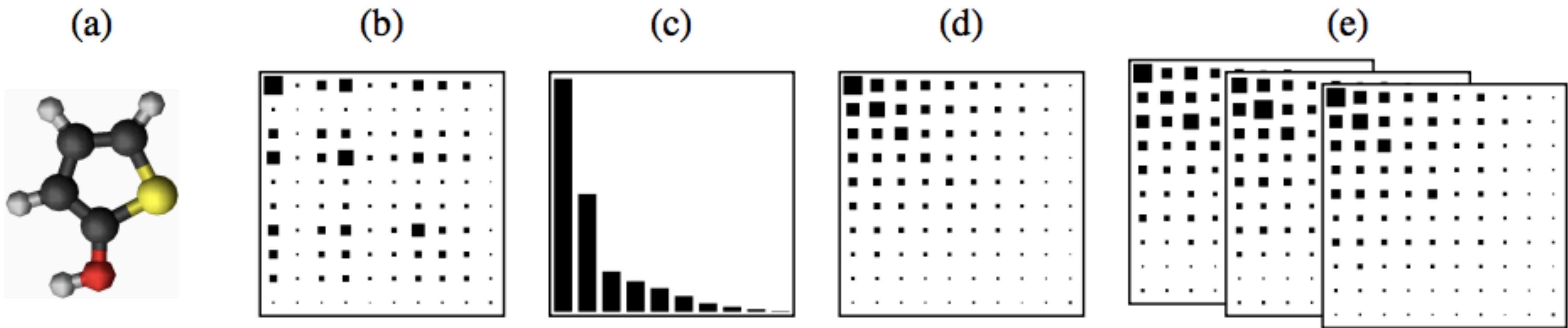
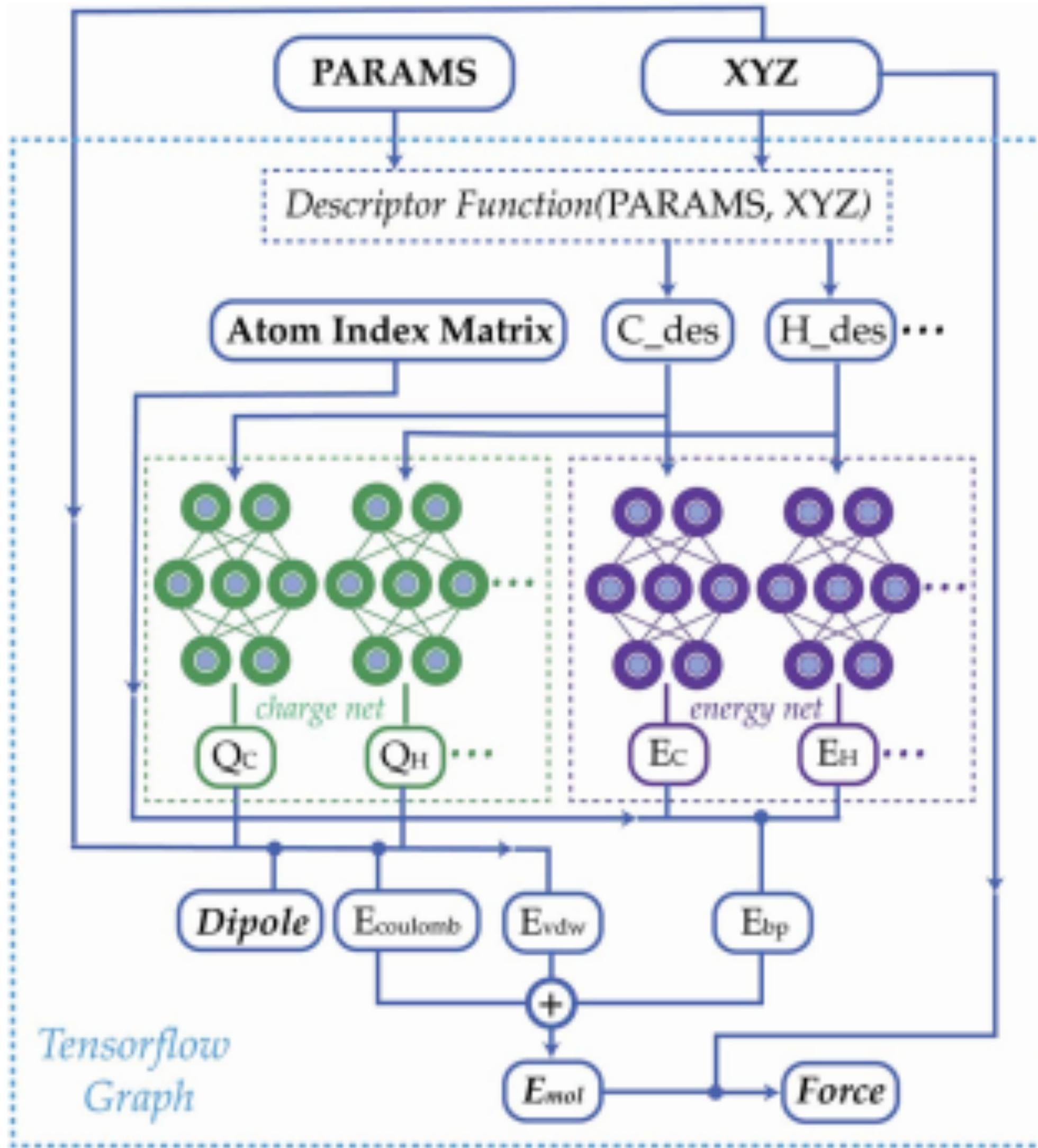


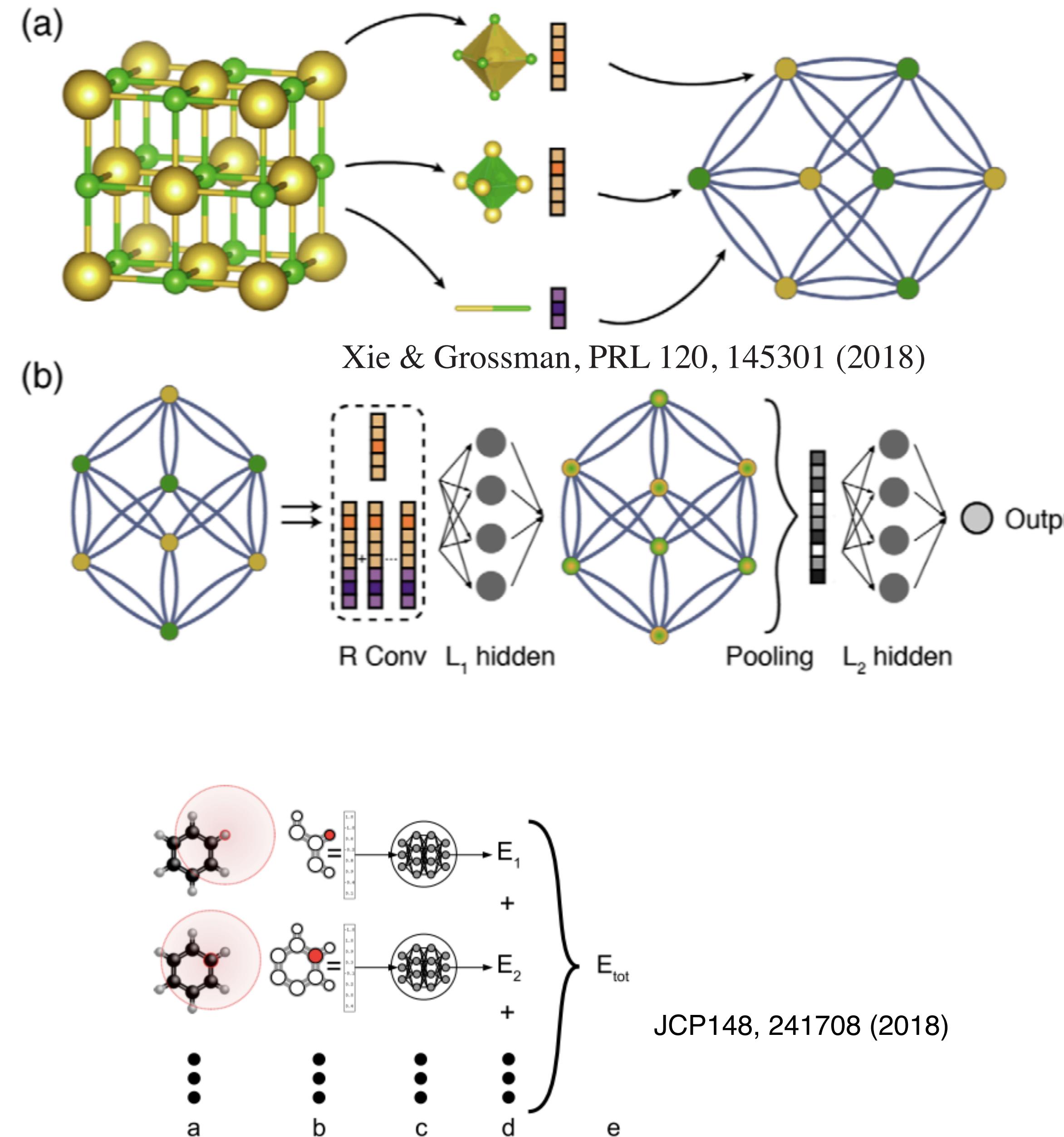
Figure 1: Different representations of the same molecule: (a) raw molecule with Cartesian coordinates and associated charges, (b) original (non-sorted) Coulomb matrix as computed by Equation 1, (c) eigenspectrum of the Coulomb matrix, (d) sorted Coulomb matrix, (e) set of randomly sorted Coulomb matrices.

arXiv:1711.06385v2



TensorMol

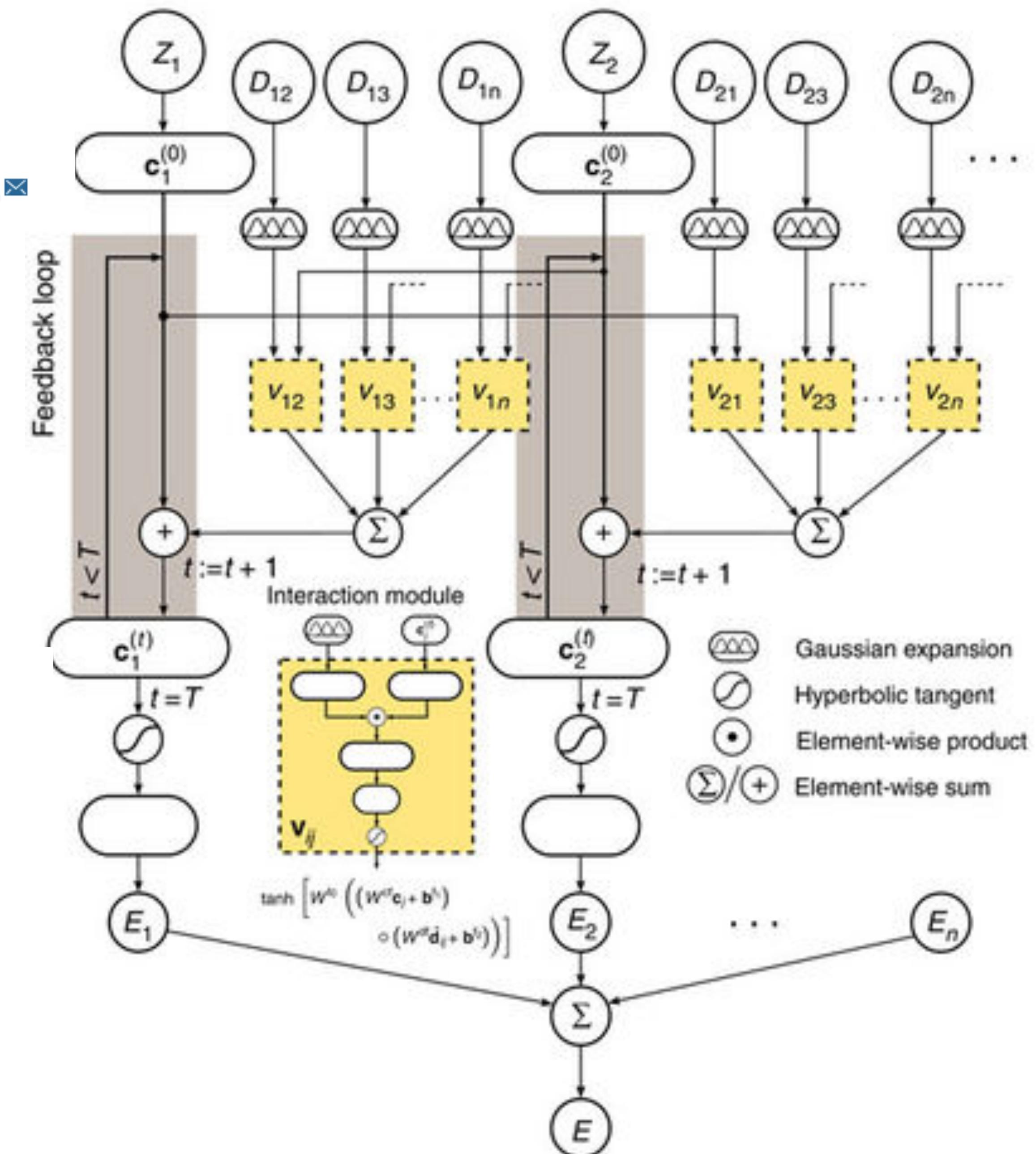
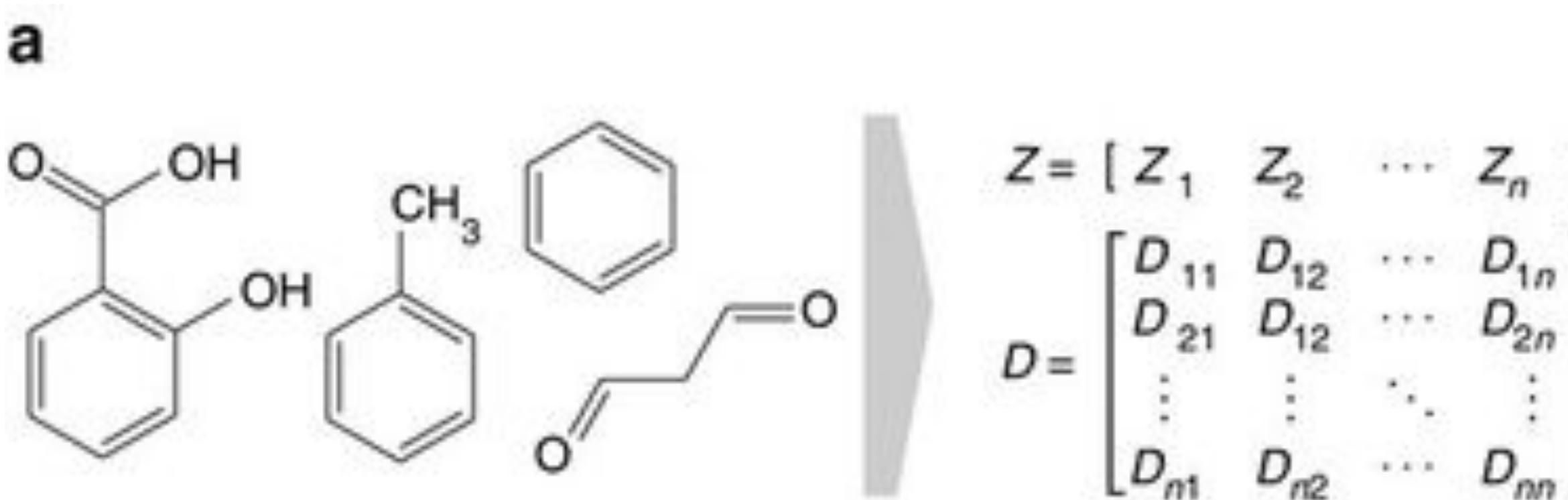
Convolutional graph



Quantum-chemical insights from deep tensor neural networks

Kristof T. Schütt, Farhad Arbabzadah, Stefan Chmiela, Klaus R. Müller & Alexandre Tkatchenko

Nature Communications 8,
Article number: 13890 (2017)
doi:10.1038/ncomms13890



DTNN

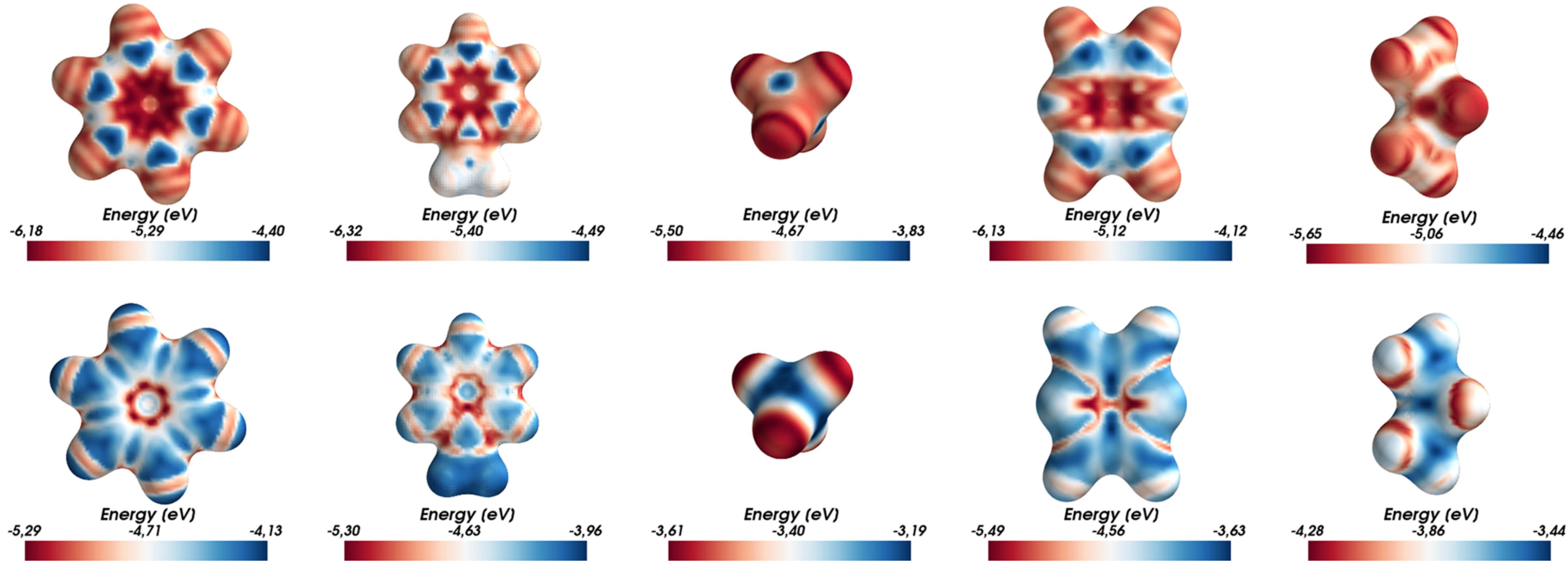


FIG. 5. Local chemical potentials $\Omega_C(\mathbf{r})$ of DTNN (top) and SchNet (bottom) using a carbon test charge on a $\sum_i \|\mathbf{r} - \mathbf{r}_i\| = 3.7 \text{ \AA}$ isosurface are shown for benzene, toluene, methane, pyrazine, and propane.

...and materials!

ARTICLE

doi:10.1038/nature25978

Planning chemical syntheses with deep neural networks and symbolic AI

Marwin H. S. Segler^{1,2}, Mike Preuss³ & Mark P. Waller⁴

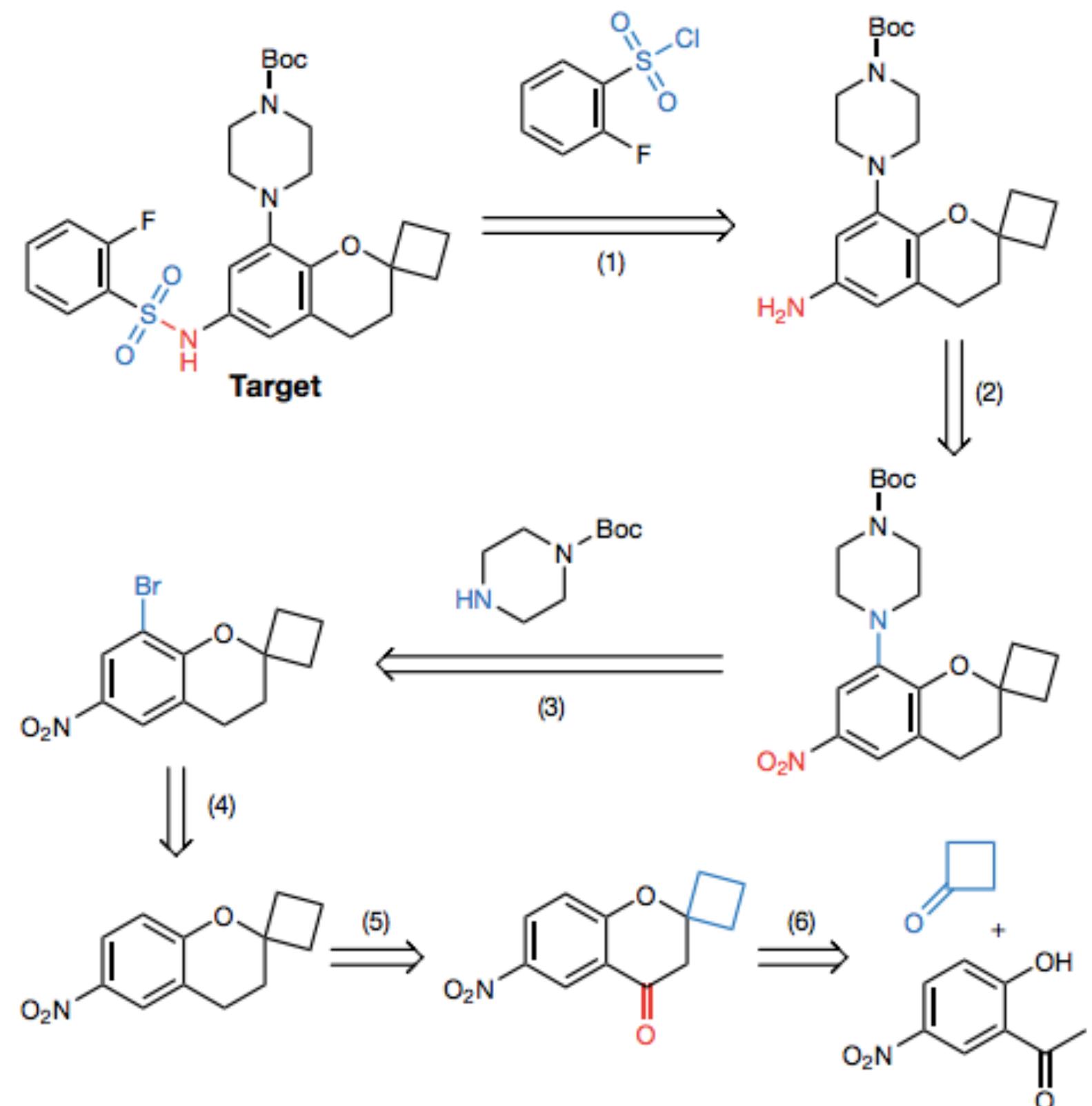


Figure 3 | An exemplary six-step synthesis route for an intermediate in a drug candidate synthesis. This route is identical to the published one⁴⁴ and was found by our algorithm autonomously within 5.4 s. The affected functional groups in each step are marked blue or red.

To address surface reaction network complexity using scaling relations machine learning and DFT calculations

Zachary W. Ulissi, Andrew J. Medford, Thomas Bligaard & Jens K. Nørskov

Nature Communications 8,

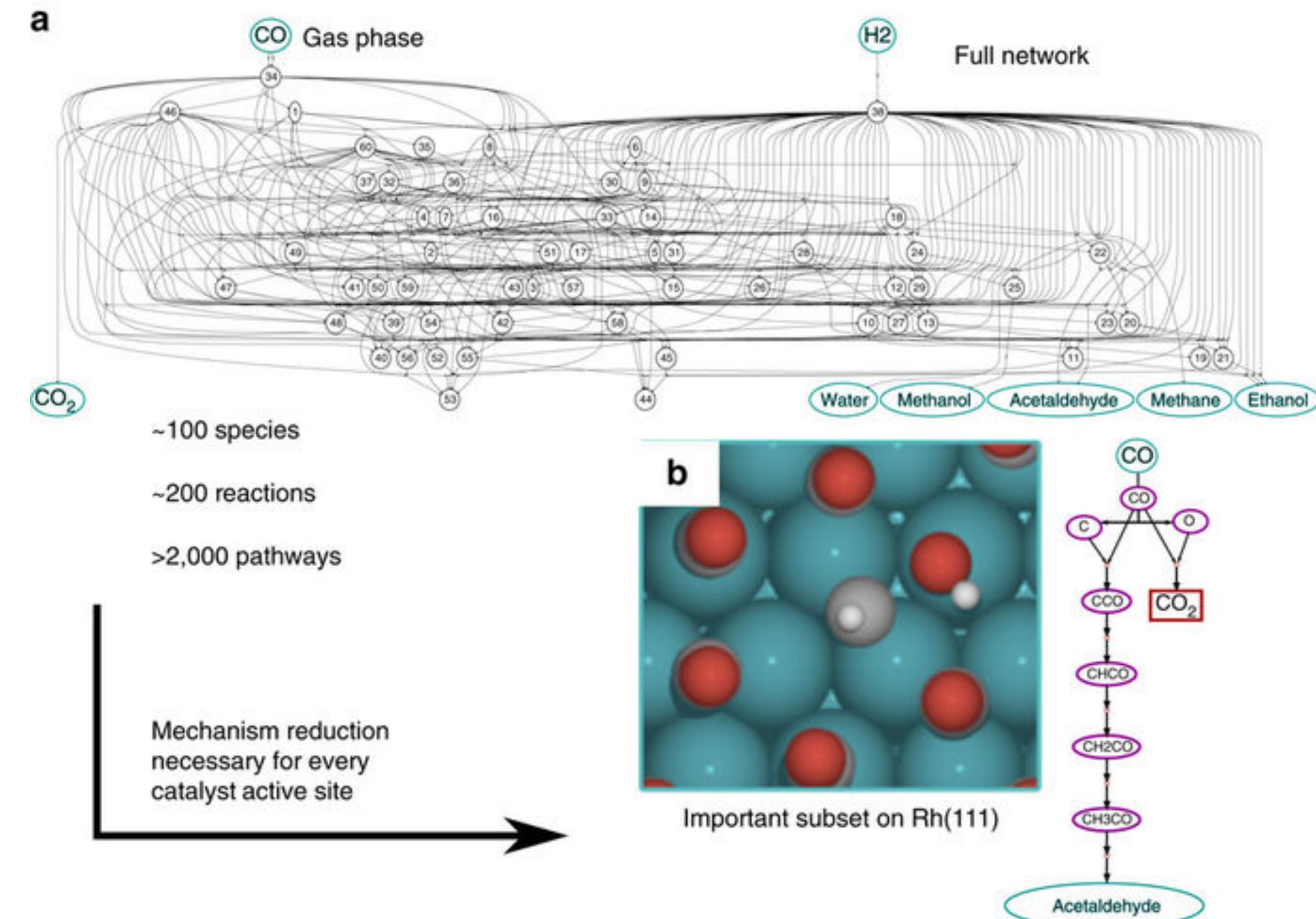
Article number: 14621 (2017)

doi:10.1038/ncomms14621

Received: 11 October 2016

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Published: 06 March 2017



AI

Collaborative
elements

Material synthesis,
characterization,
design

Physical theory,
simulation,
modelling

A Multi-scale Modeling Framework for Advanced CO₂ Conversion Electrocatalysts

RHEINISCHE
WESTFÄLISCHE
TECHNISCHE
HOCHSCHULE
AACHEN



RWTH

PIs (RWTH/Julich): Prof. Olivier Guillon, Prof. M. Eikerling

PI (NRC): Kourosh Malek

Team: Stefan Baumann, Wendelin Deibert (Julich),

Qianpu Wang, Ali Malek (NRC)

Gagandeep Sing Bajwa (Coop Student)

Motivation, Objective, Deliverables

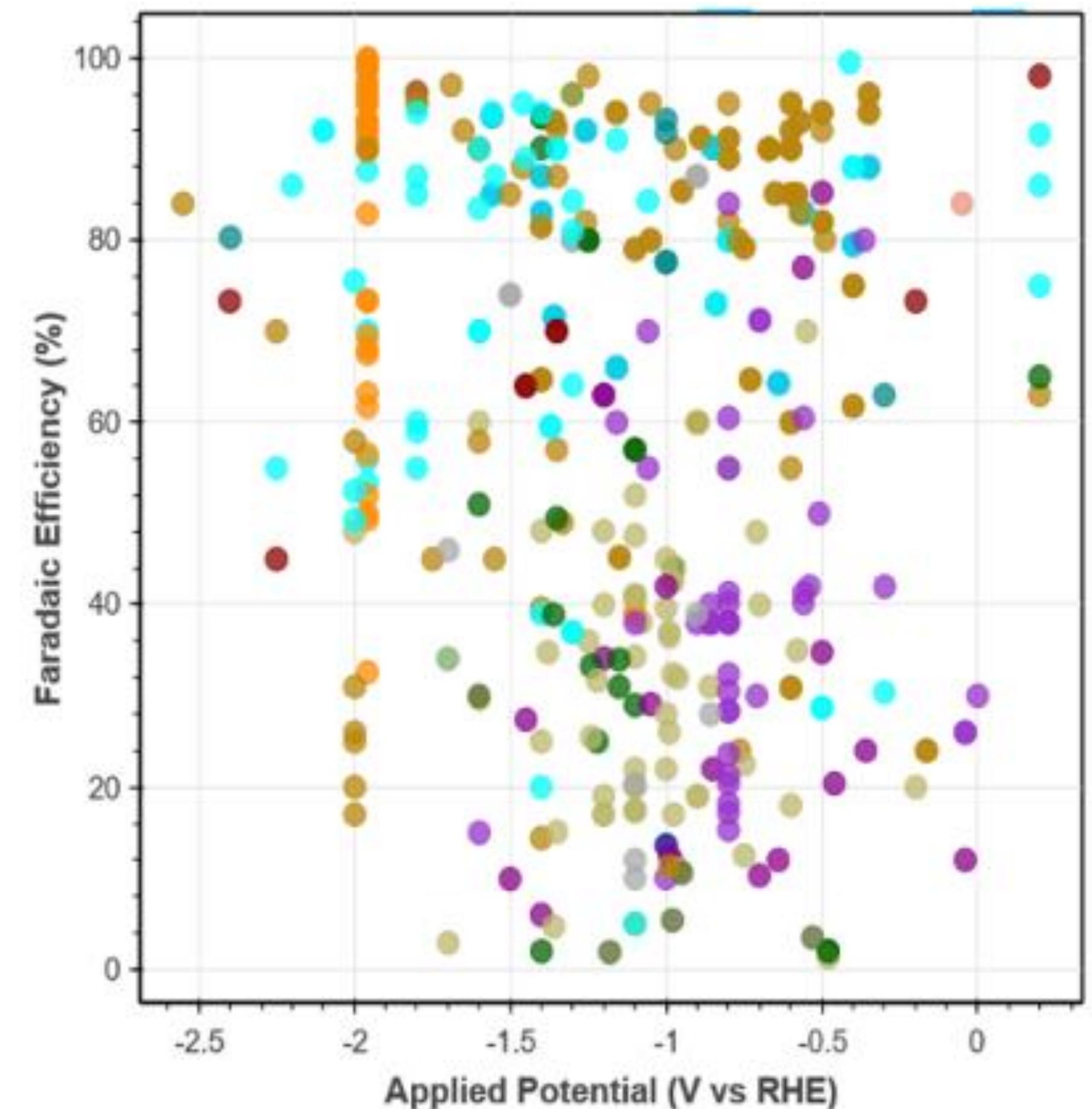
A data-driven framework (modeling/experiment) towards understanding reaction mechanisms and pathways that determine catalyst activity and selectivity of CO₂ conversion at low & high temperatures

- To develop a comprehensive micro-kinetics model based on available modeling and experimental data for a representative set of reaction mechanisms and pathways
- Develop a comprehensive database for CO₂ electrocatalysts
- Deploy ML/DL algorithms to rationalize and predict the effect of electrode materials on activity and product selectivity

Key Deliverables

Phase 1: Database and predictive data models

Phase 2: Micro kinetics model and analysis

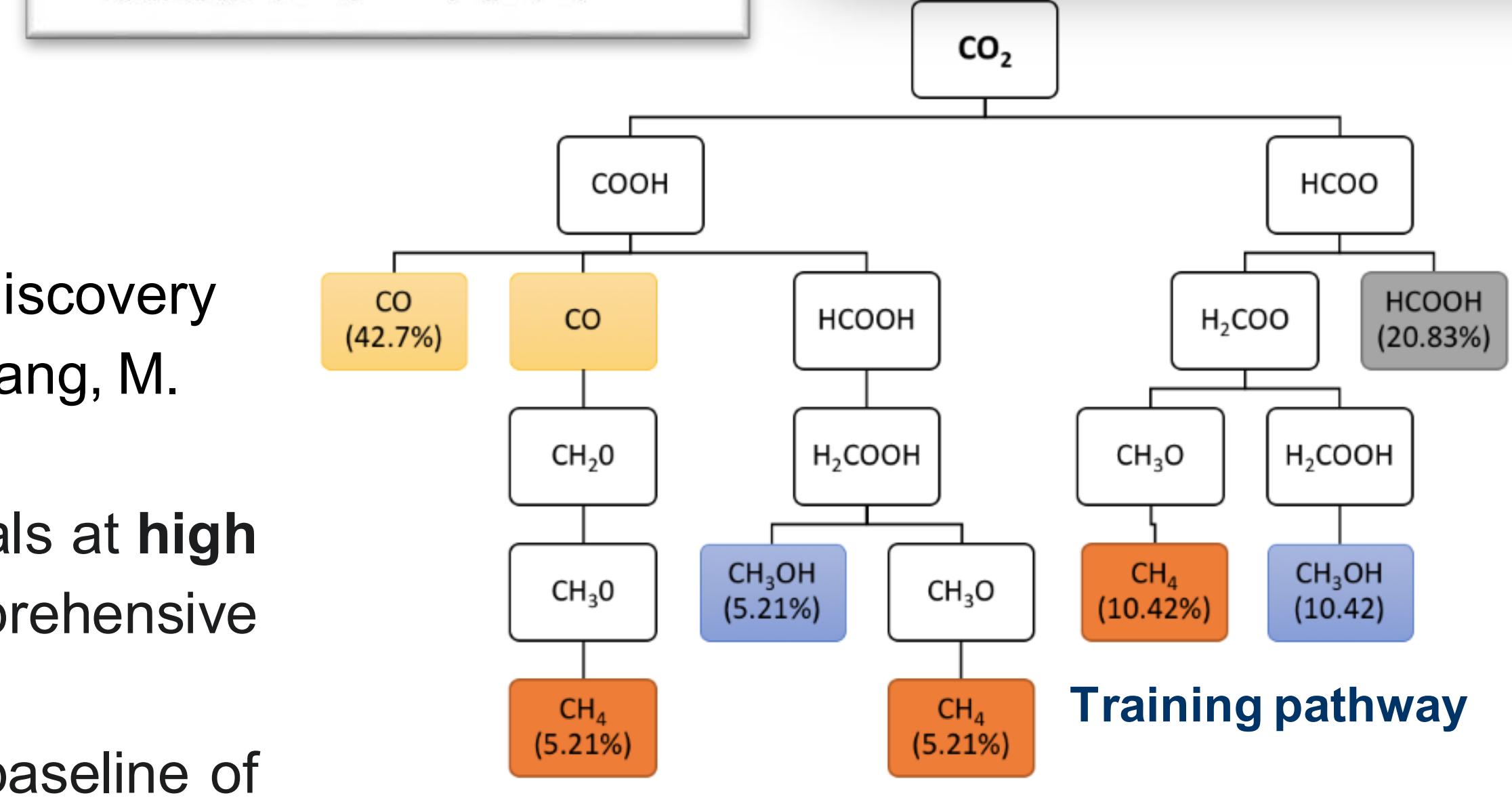
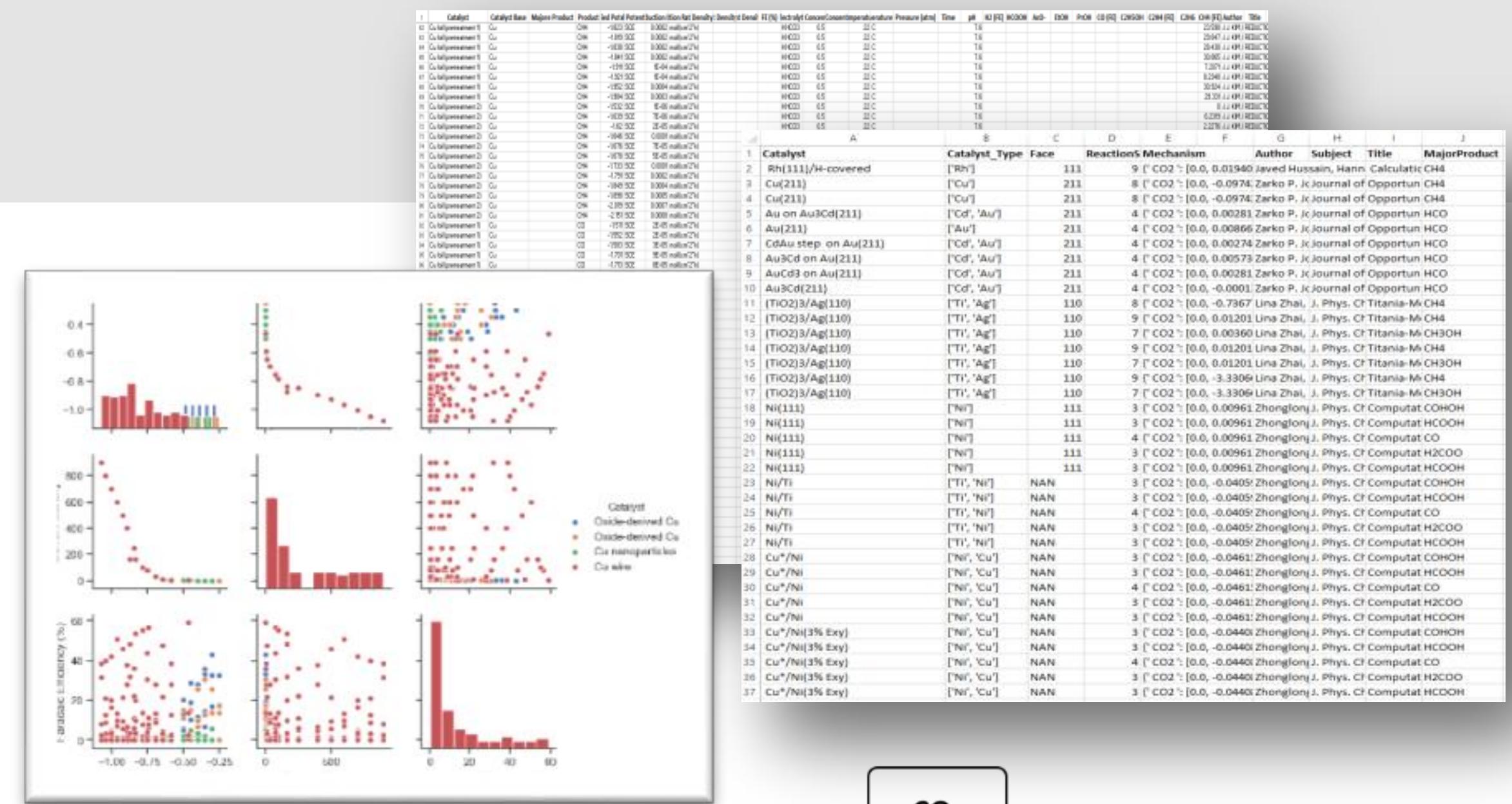


Summary of activities

Phase 1 completed

> 400 references for Low-T catalytic materials = 1200 data points (experimental/computational)

- Target & performance attributes are defined
- Studied product selectivity for
 - HCOOH, CO, HCOO
- Predictive & optimization models (selectivity, yield, activity)
- Cu₂O, **Cu-MO Loaded**, ZnO, G



An Integrated Acceleration Platform for Membrane Electrode Assembly + Foundational Infrastructure



PIs (UBC): Jason Hein, Curtis Burlingette

PI (NRC): Kourosh Malek

NRC Team: Robert Black, Ken Shi, Qianpu Wang, Ali Malek,
Zhong Xie

Jenya Sourgaeva (Coop Student)

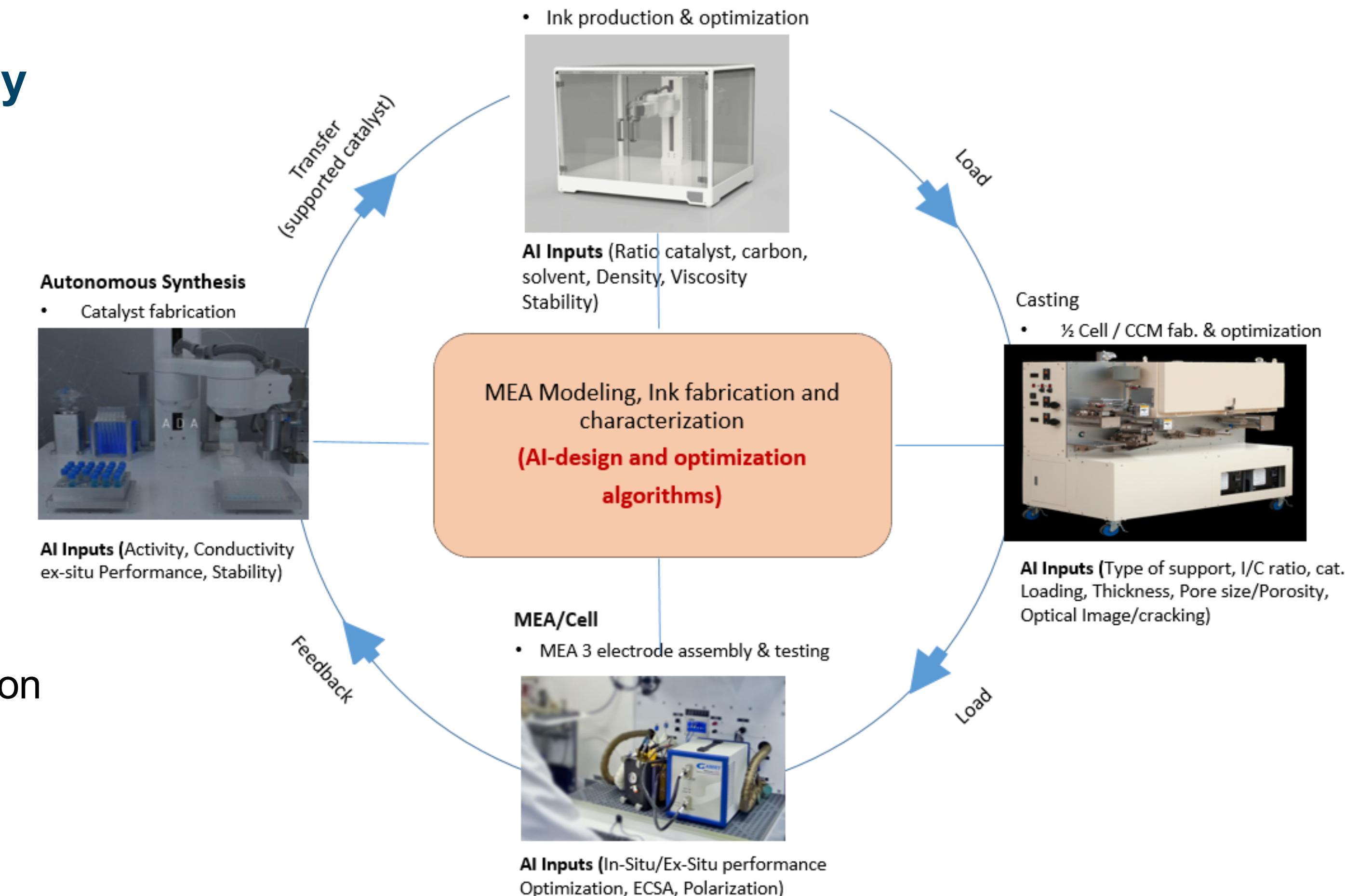
Motivation, Objectives, Deliverables

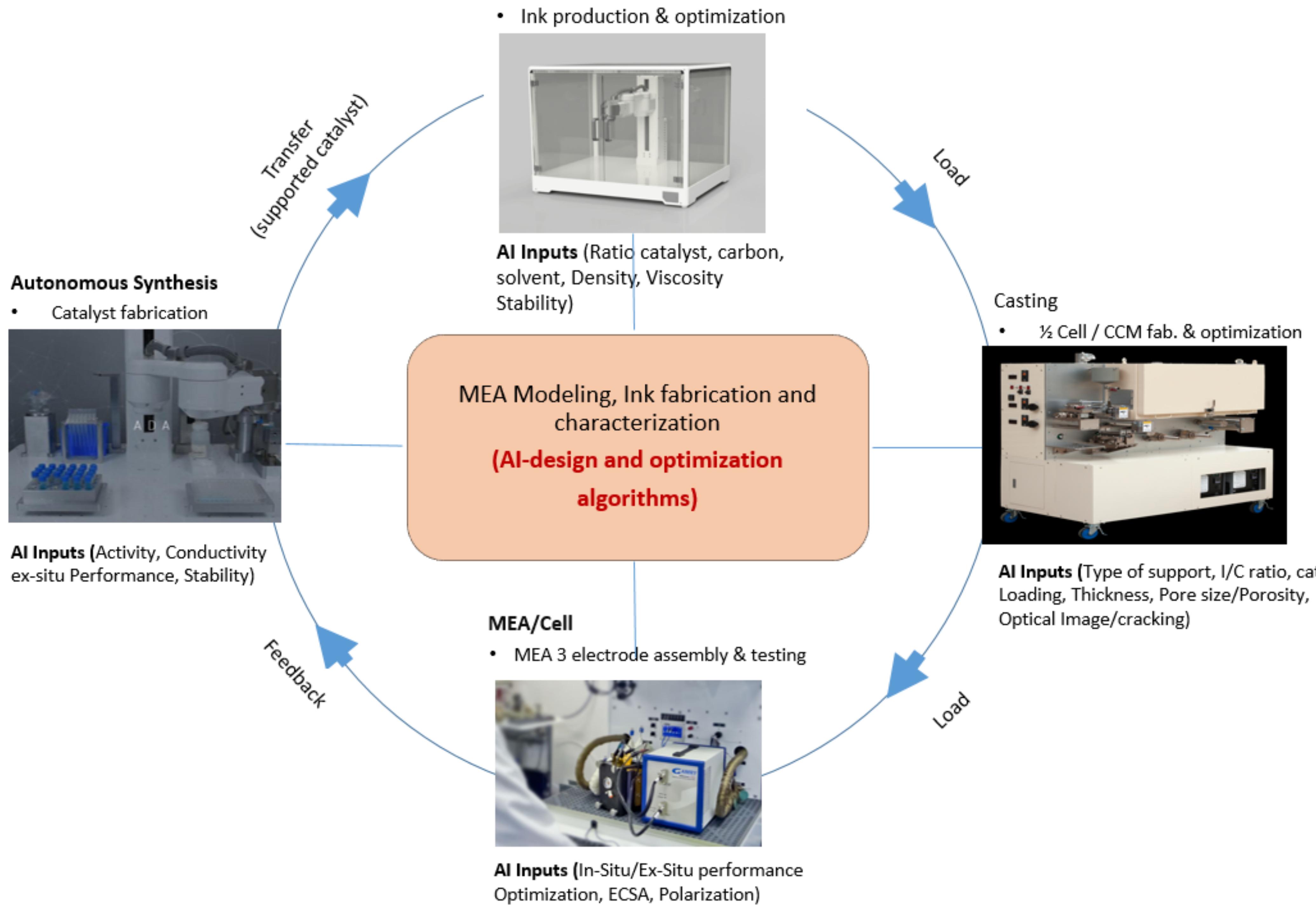
An Integrated Design and Optimization Framework for Membrane Electrode Assembly (MEA) & Catalyst Coated Membrane (CCM)

- Specific focus on CO₂ conversion and H₂ electrolysis
- Collecting modeling and experimental data relevant to optimization of the ink composition and fabrication
- Apply **self-learning algorithms** to predict insights into MEA design fabrication & optimization

Key Deliverables

- A modular data-driven framework to be used for preliminary ink fabrication guidelines
- Established baseline ink formulation for CCM fabrication
- Optimization framework for GDL/MEA (March 2021)
- End-to-end workflow management and MEA Scale up



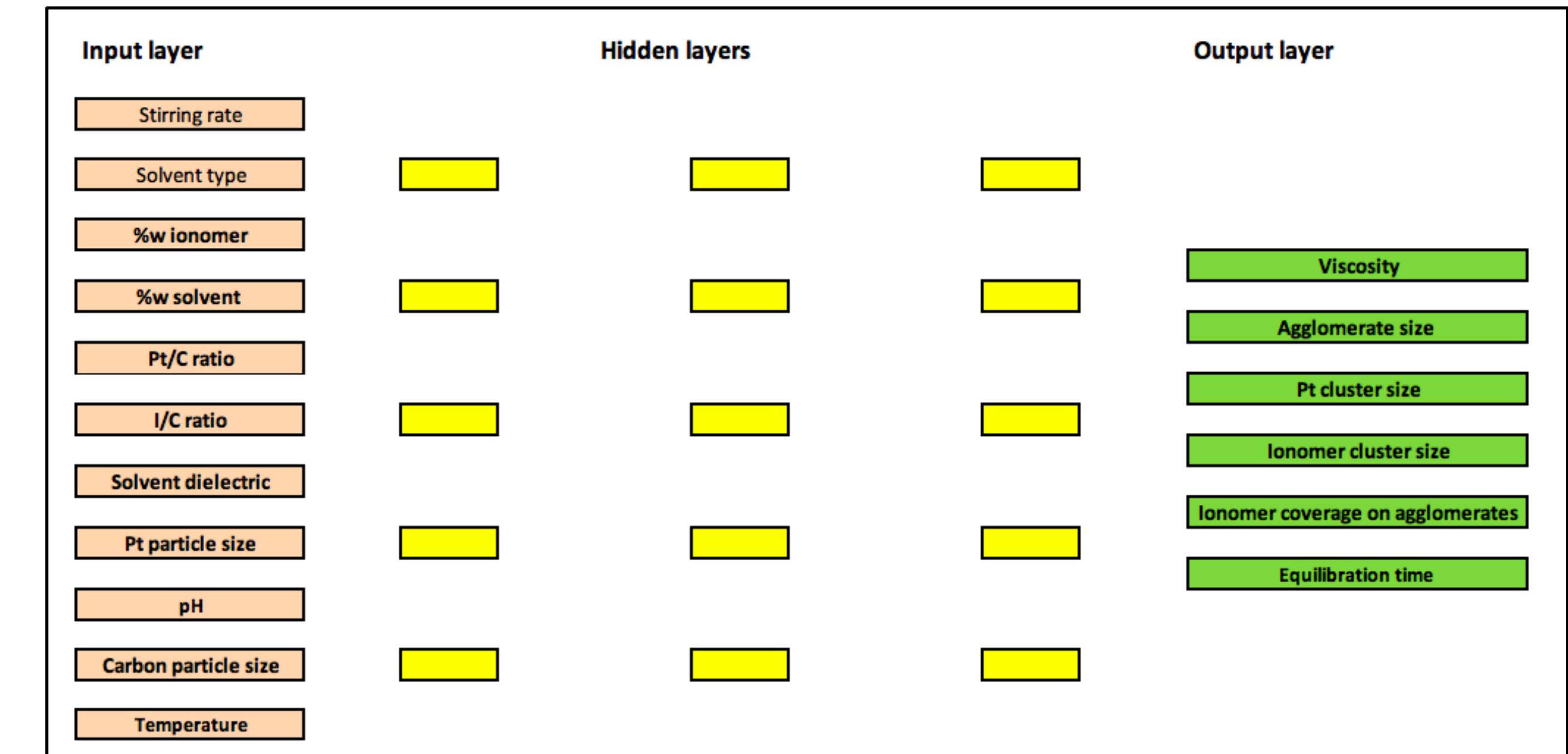


Summary of activities

Kick-off meeting was held on April 28, 2020

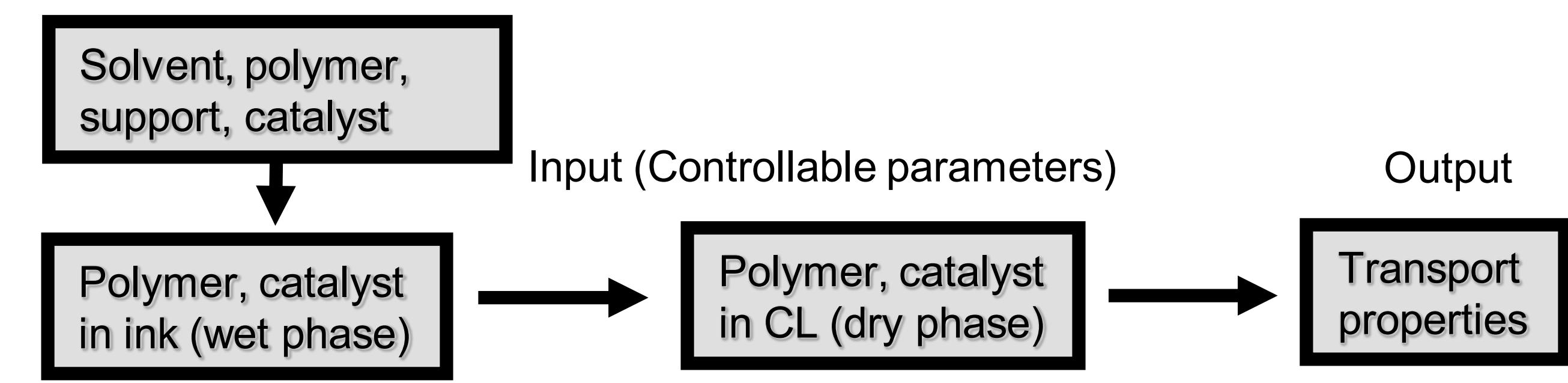
Current activities

- Preparing training, validation & test data-sets
- Developing data models / structure
- Defining descriptors at **ink preparation stage**
- Supporting UBC's new MEA-MAP infrastructure



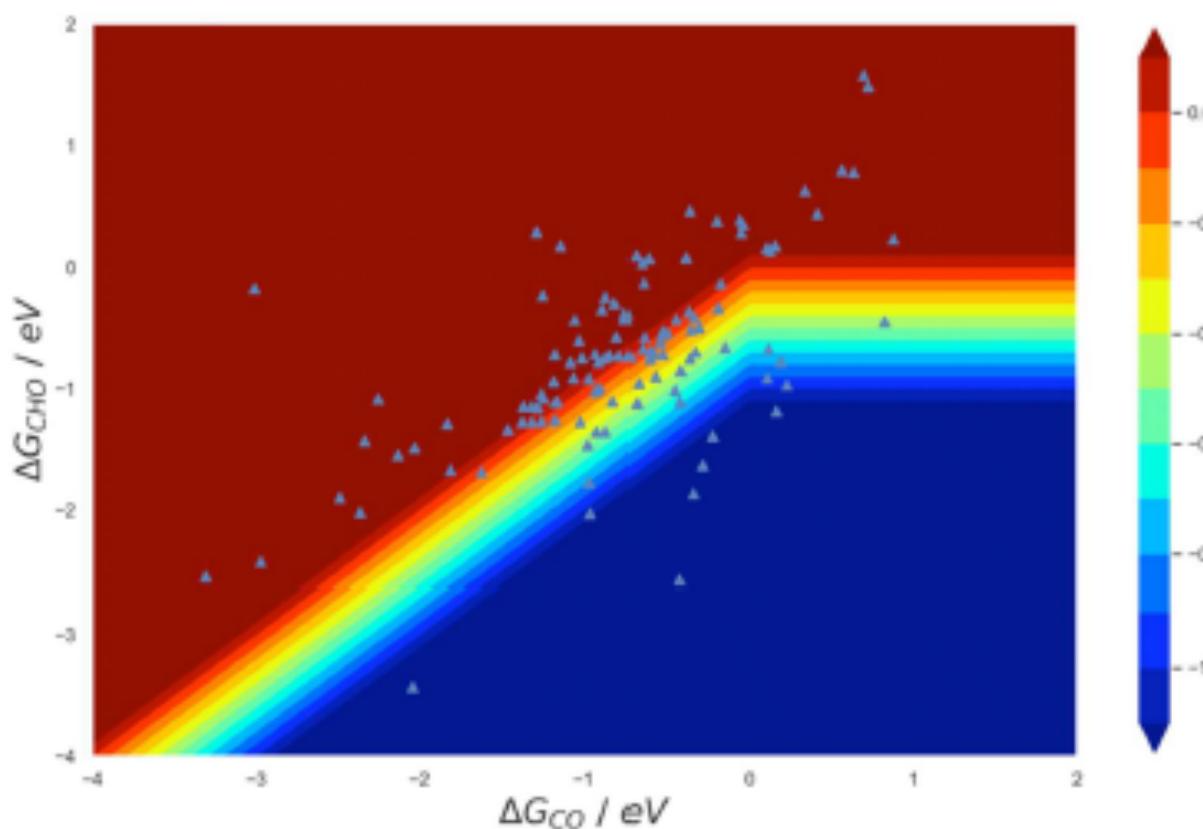
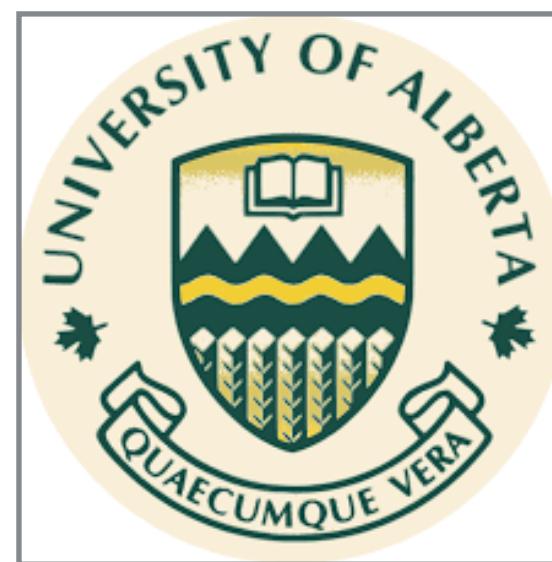
Ongoing tasks

- Collecting baseline ink composition & MEA performance-durability testing data
- Cross-checking, validation and optimization
- Developing ML algorithms / predictive models



Prof. Samira Siahrostami (UofC)

Catalyst Development for CO₂ Conversion to Value-added Chemicals
Using Combined DFT/ML and Experiment



Dr. Sergey Gusarov (NRC)
Dr. Stanislav Stoyanov (CanMet, UofA)

Applicant Highlights

- Early career professor trained by Jens Norskov at Stanford University (pioneer in computational catalysis)
- Expert in quantum-mechanical simulations for electrocatalysis

Activities

- DFT calculations on perovskites and transition metal nitrides
- Machine learning algorithm development with neural networks
- Catalyst synthesis and validation



We aim to perform robust **high throughput DFT** calculations to screen large search space of **metal oxides** and **metal nitrides** for CO₂RR. Our screening results will be used as datasets in order to develop ML methods to accelerate **catalyst materials discovery**. To this end, we aim to develop and use ML models that include **orbitals interactions features** as well as features that include electronic structure attributes such as **Fukui Function** when representing catalyst materials for adsorption energies prediction. Very recently, we developed a ML model by including orbitals interactions for predicting properties of crystalline systems such as formation energy, Fermi energy and band gap. Our developed novel model, Orbital Crystal Graph Convolutional Neural Network (OGCNN), significantly outperforms recently developed Crystal Graph Convolutional Neural Network (CGCNN) model by at least 60 % in accuracy prediction. The success of this novel CGCNN model is due to incorporation of orbital interaction features for the first time. In this proposal, we take the **OGCNN** model one step further to predict binding energies of adsorbates on catalysts materials.

¹ Development of Fukui Function Based Descriptors for a Machine Learning Study of CO₂ Reduction

³ Sergey Gusarov,* Stanislav R. Stoyanov, and Samira Siahrostami



Cite This: <https://dx.doi.org/10.1021/acs.jpcc.0c03101>



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ACCESS |

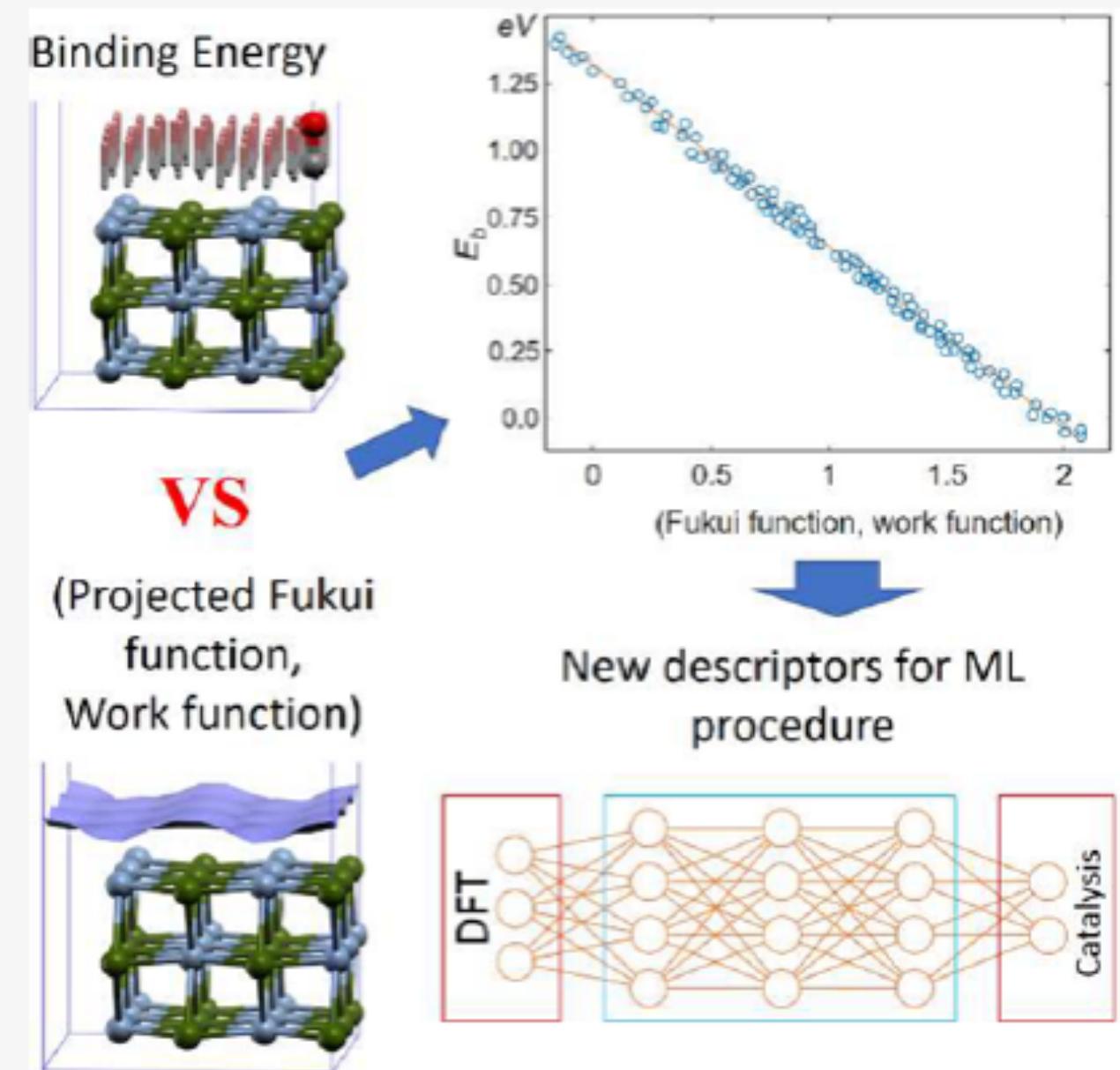


Metrics & More

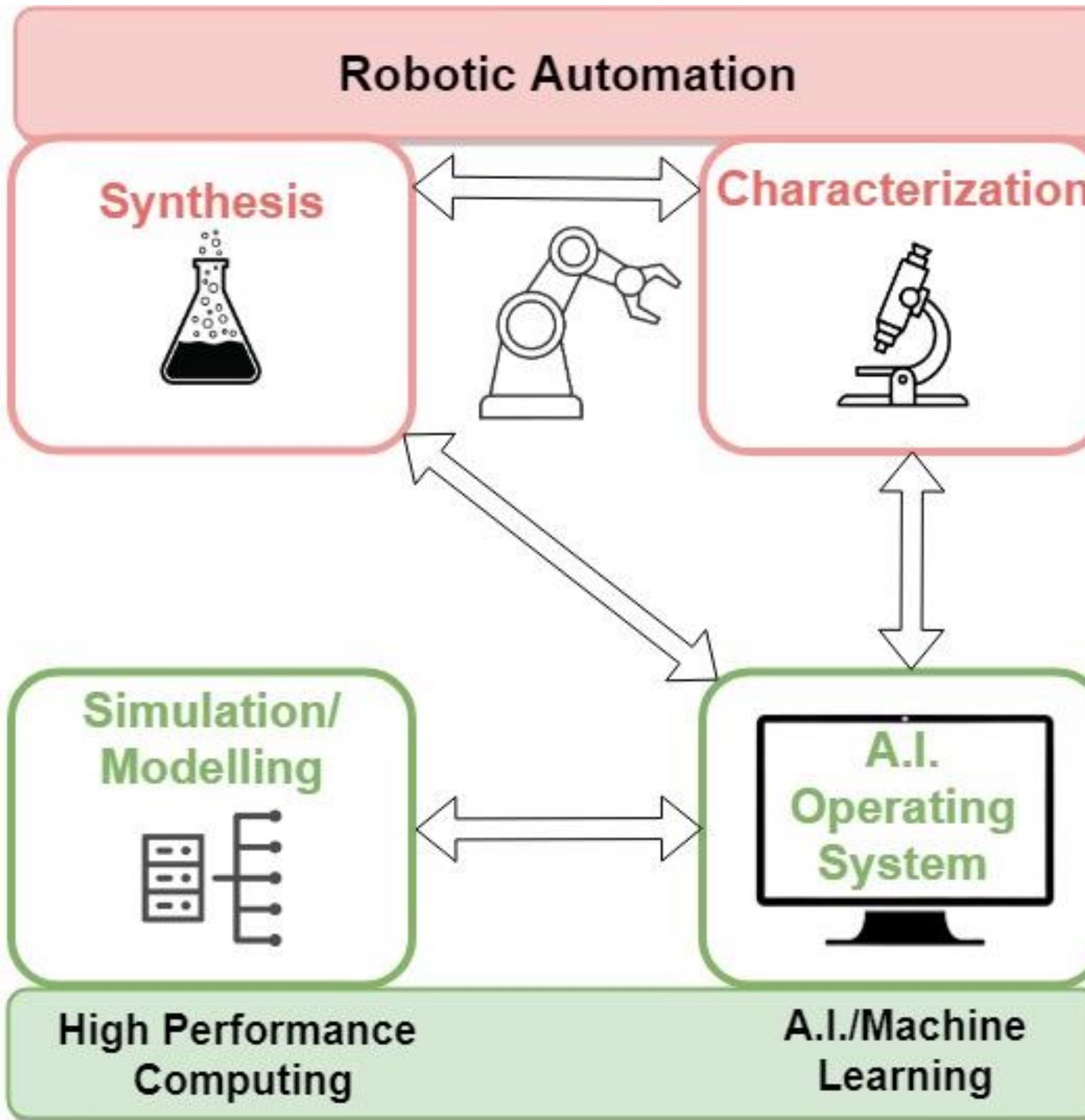


Article Recommendations

⁴ **ABSTRACT:** Developing novel methods that capture chemical properties quickly and with reasonable accuracy has emerged as an attractive way to replace time-consuming density functional theory (DFT) calculations. In this study, we propose a new type of machine learning (ML) enhanced descriptors based on the Fukui function (FF) projected onto the Connolly surface. The FF contains information about the local system's response to the perturbation and could be used as a descriptor of the chemical properties of a surfaces. We show that the FF, augmented by a general characteristic of the electronic structure of the surface, such as a work function, is well correlated to the mapped adsorption energy of CO. Therefore, this combination might replace the computationally expensive mapping of the adsorption energy of small molecules as an indicator of catalytic activity. Potential extensions of the proposed methodology are briefly discussed.



Material Acceleration Platforms (MAPs) for Material Discovery – Electrocatalysis



NORTH ROBOTICS



MCF Challenge
Program



UNIVERSITY OF
TORONTO

Start-End: Oct 2019 – Oct 2021 (Phase 1)

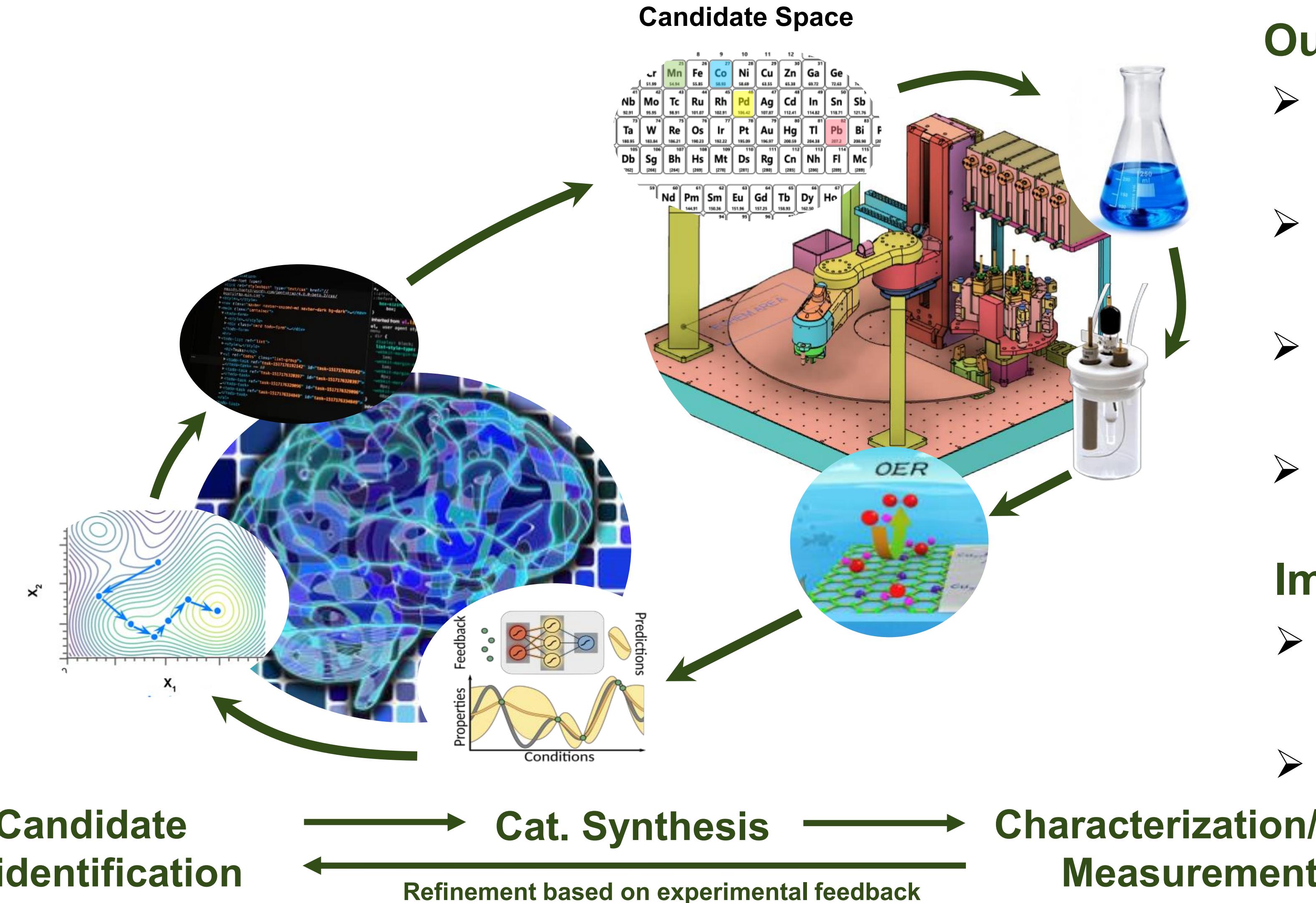
Project Leads:

Robert Black (NRC-EME Mississauga)

Zamyla Chan (Vector Institute – Alan Aspuru-Guzik)



Material Acceleration Platforms (MAPs) for Material Discovery – Electrocatalysis

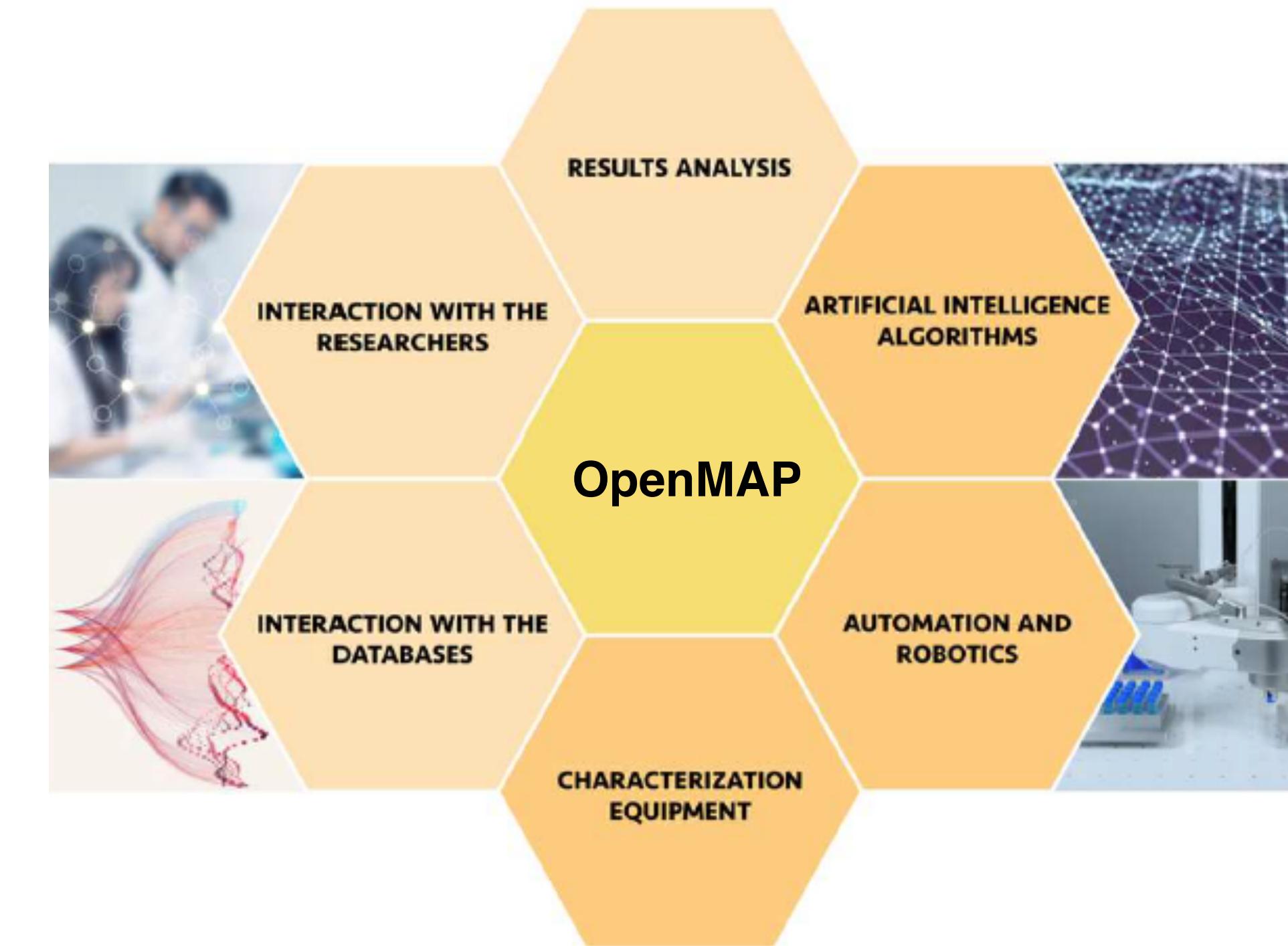


Prof. Alan Aspuru-Guzik (UofT)

OpenMAP: Self-driving laboratories

Applicant Highlights

- Pioneer in Materials Acceleration Platforms (MAPs) and co-lead on the Mission Innovation – IC 6 Clean Energy Materials
- Vector Member
- CIFAR Senior Fellow
- > 300 articles
- Multiple start-up companies



Activities

1. Extensions for inorganic materials synthesis and prediction
2. Supplying OpenMAP with robust Bayesian optimization
3. Integrating generative models into OpenMAP

Prof(s) Zack Ulissi (CMU) & Ted Sargent (UofT)

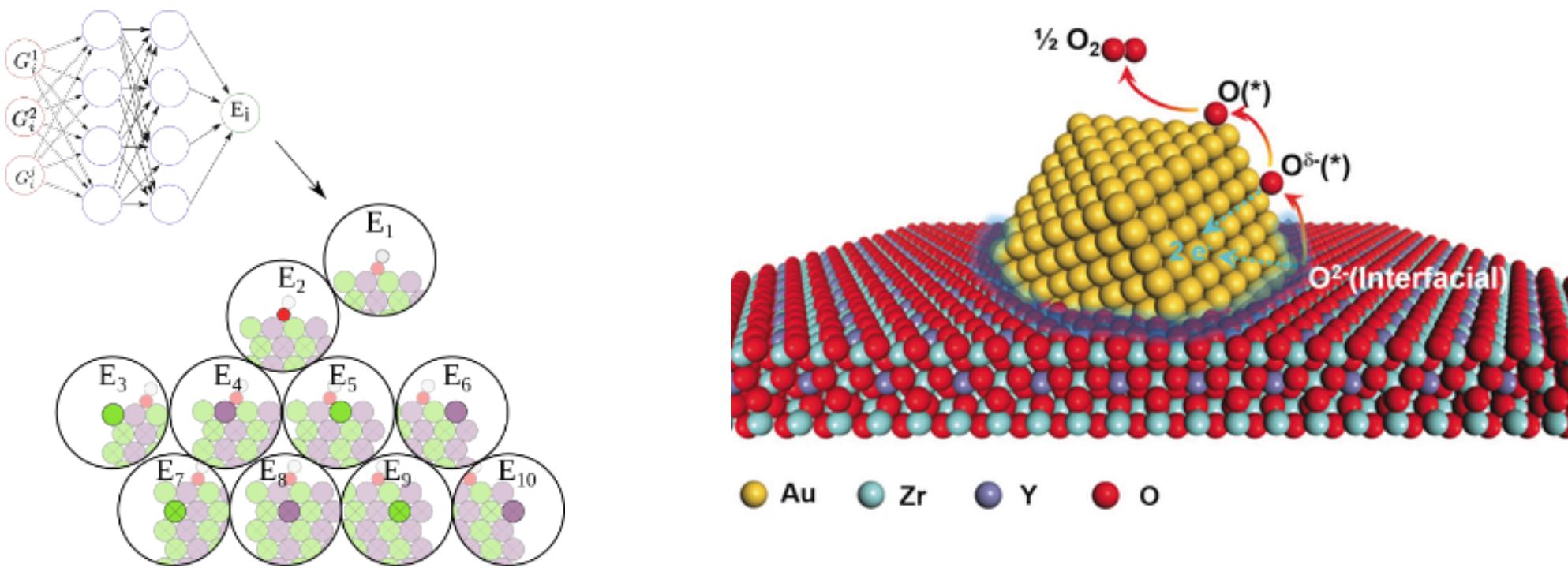
Realizing the Potential of AI/ML to Guide Experimental Discovery of Acid-Stable and PGM-Free OER Catalysts



Carnegie Mellon University

Applicant Highlights

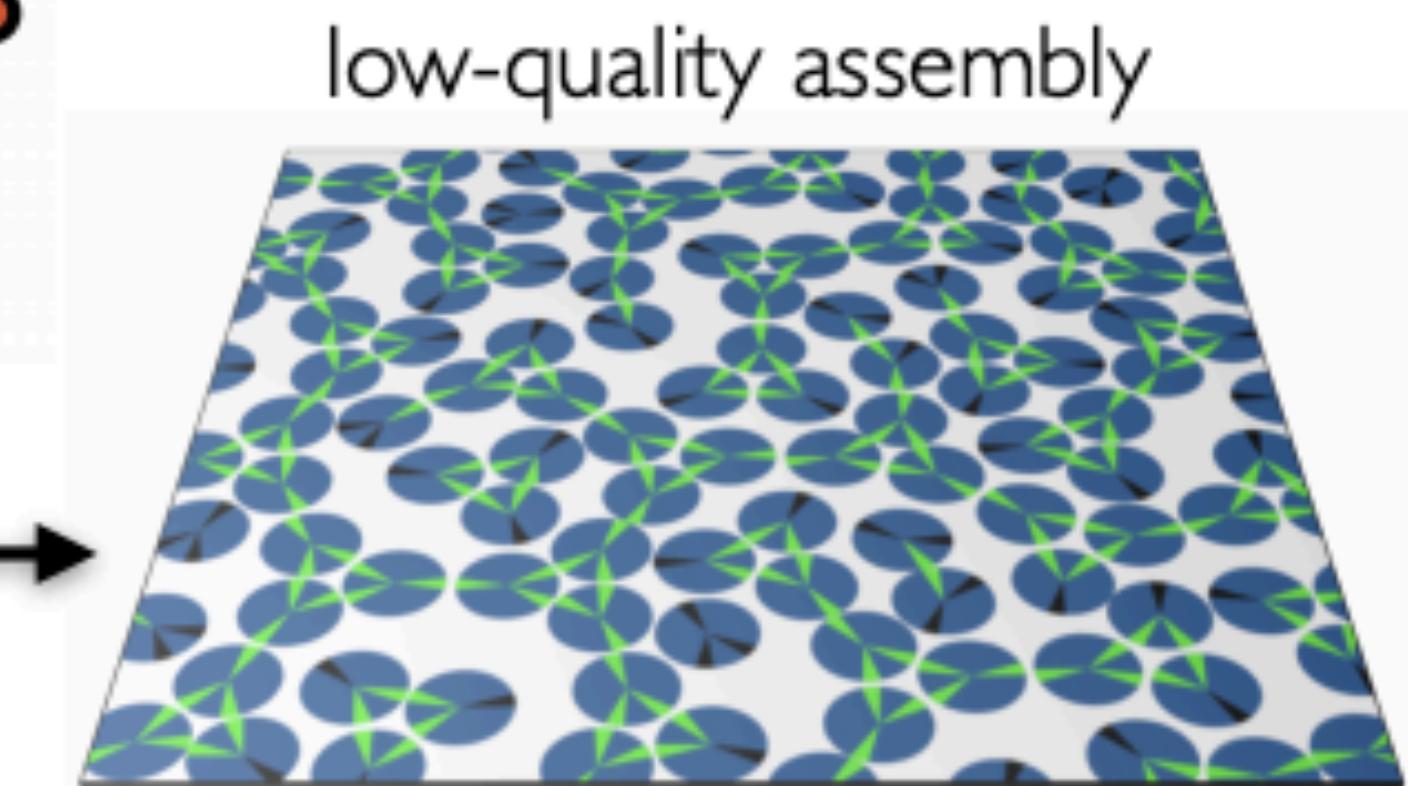
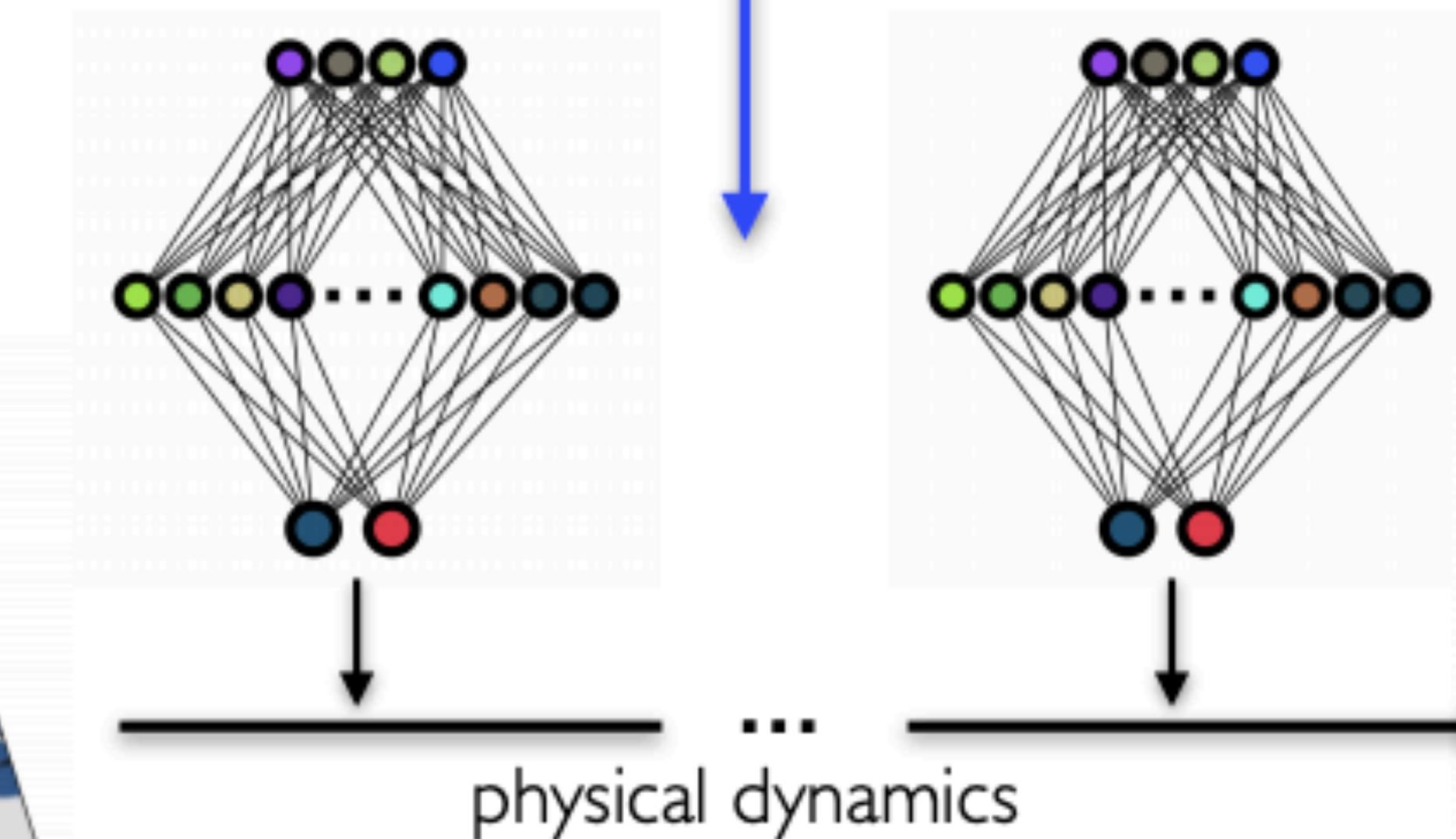
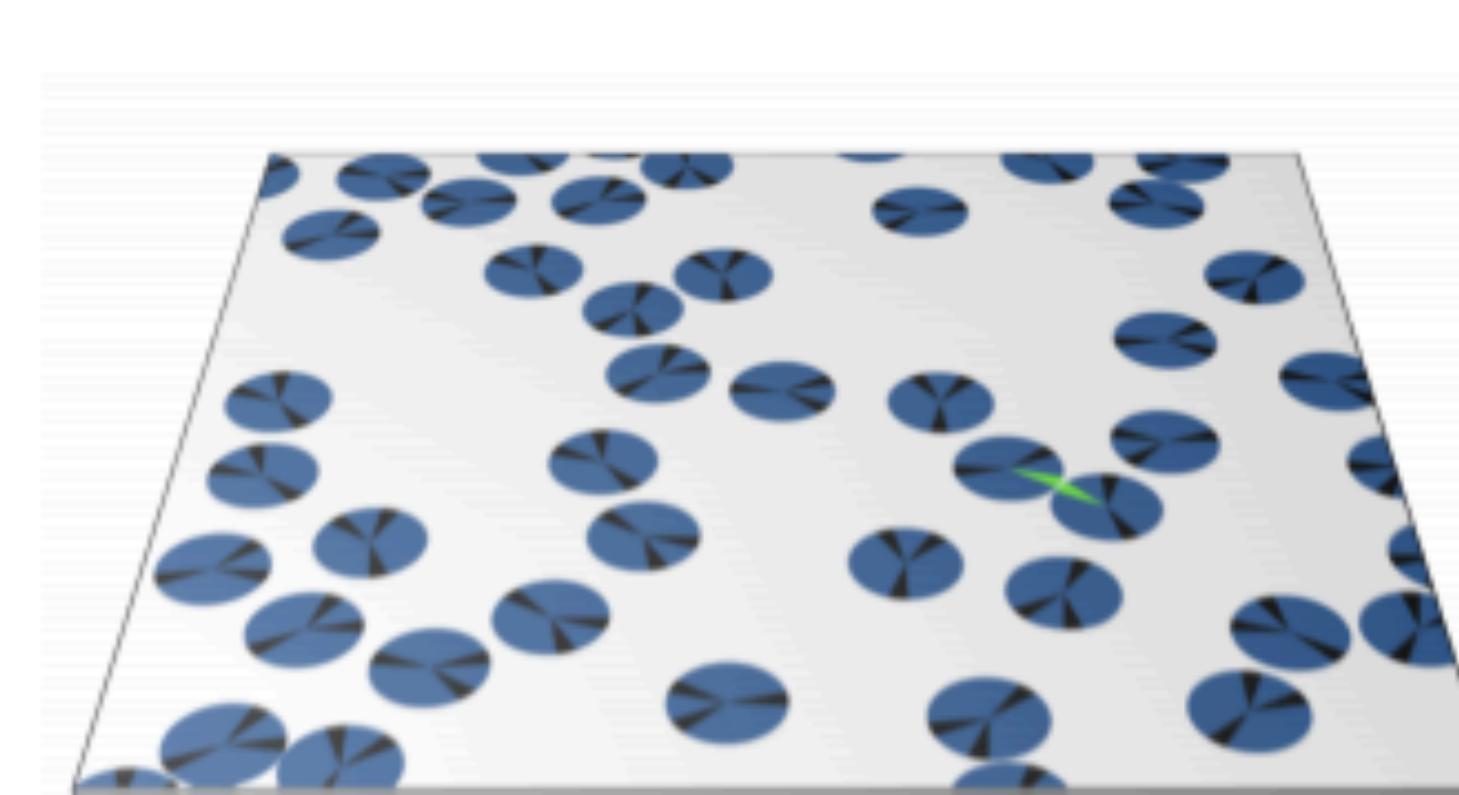
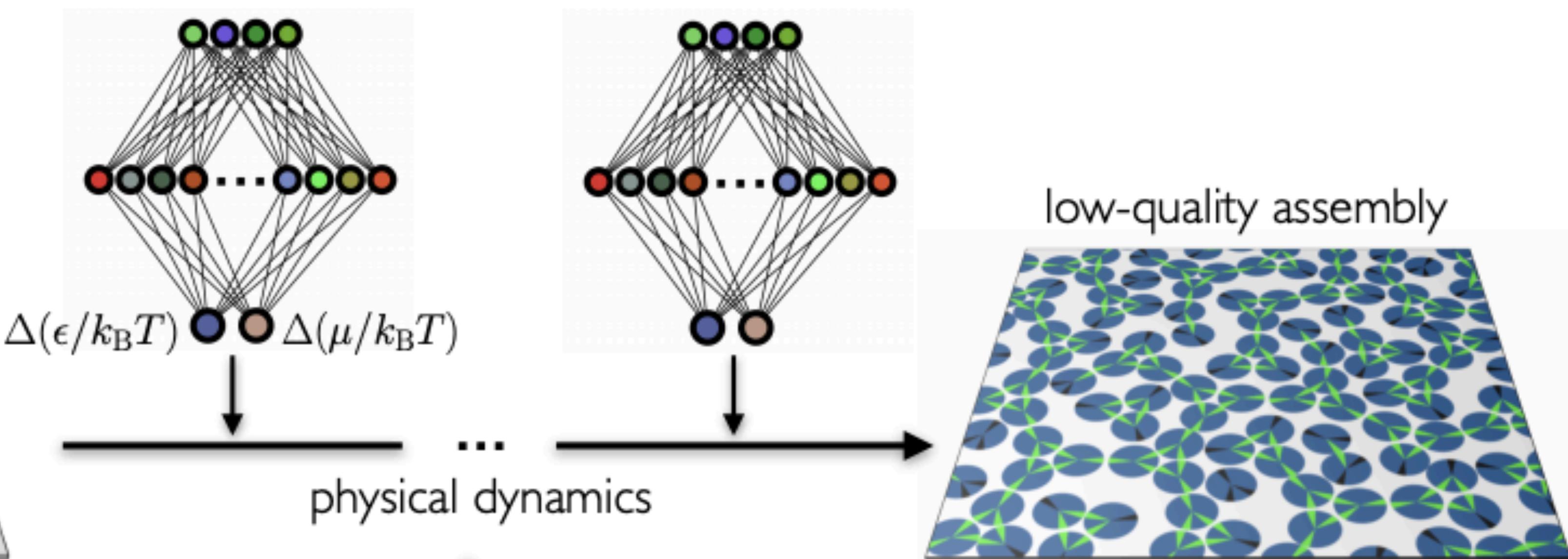
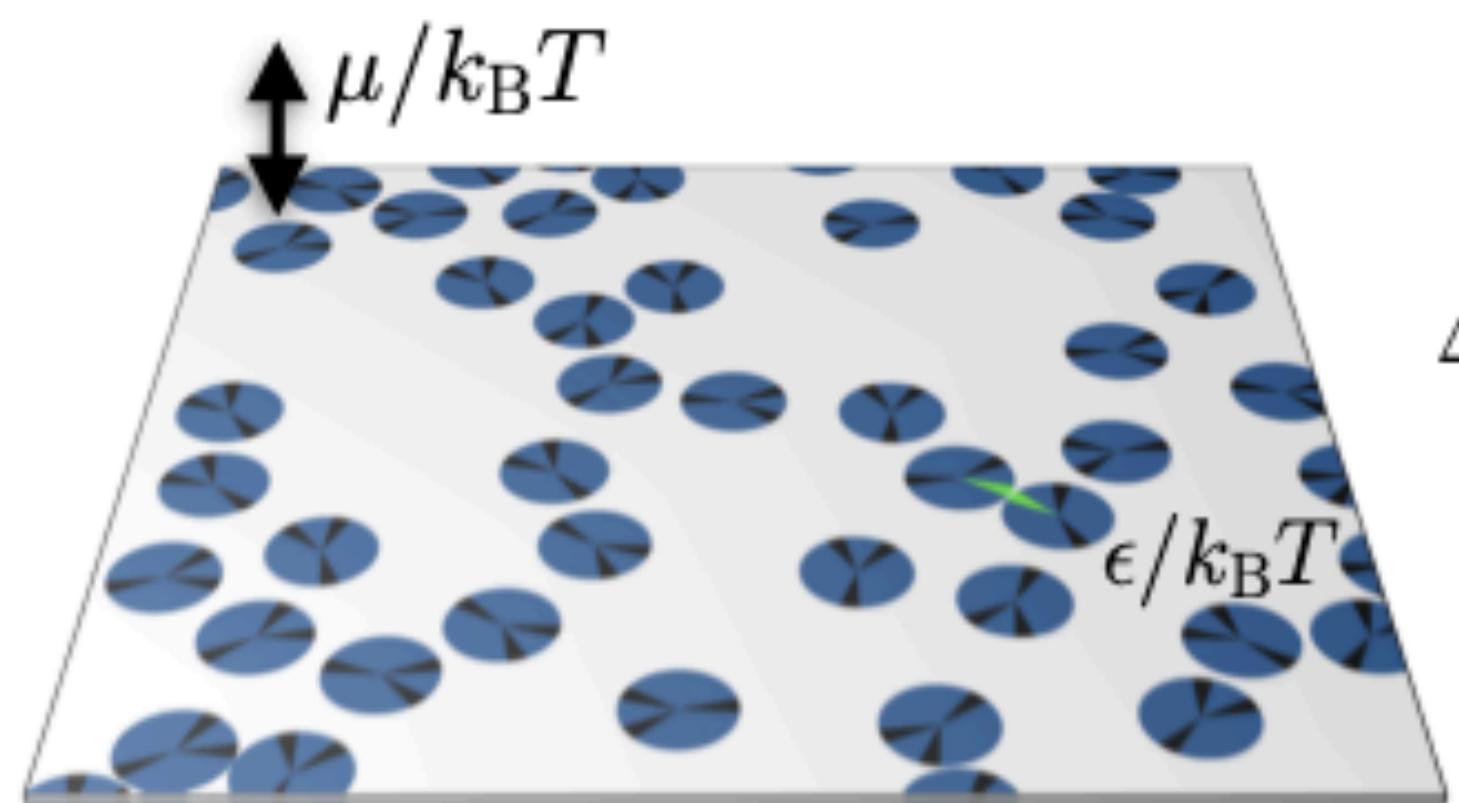
- Proposing unique HQP exchanges across 3 core sites (NRC, UofT, CMU)
- Strong coupling of established prof (Sargent) and up-and-coming prof (Ulissi)
- Integration of experimental and ML computational approaches



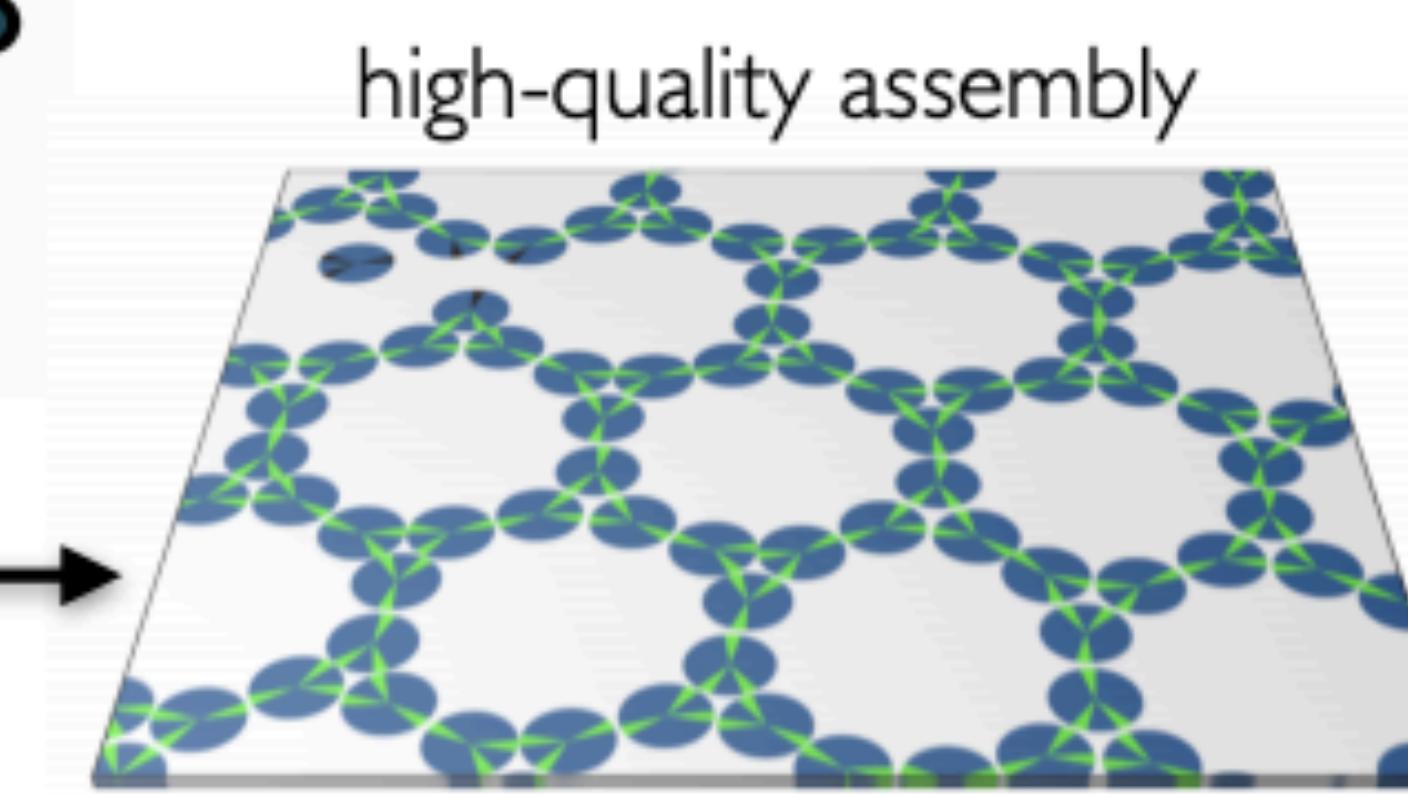
Activities

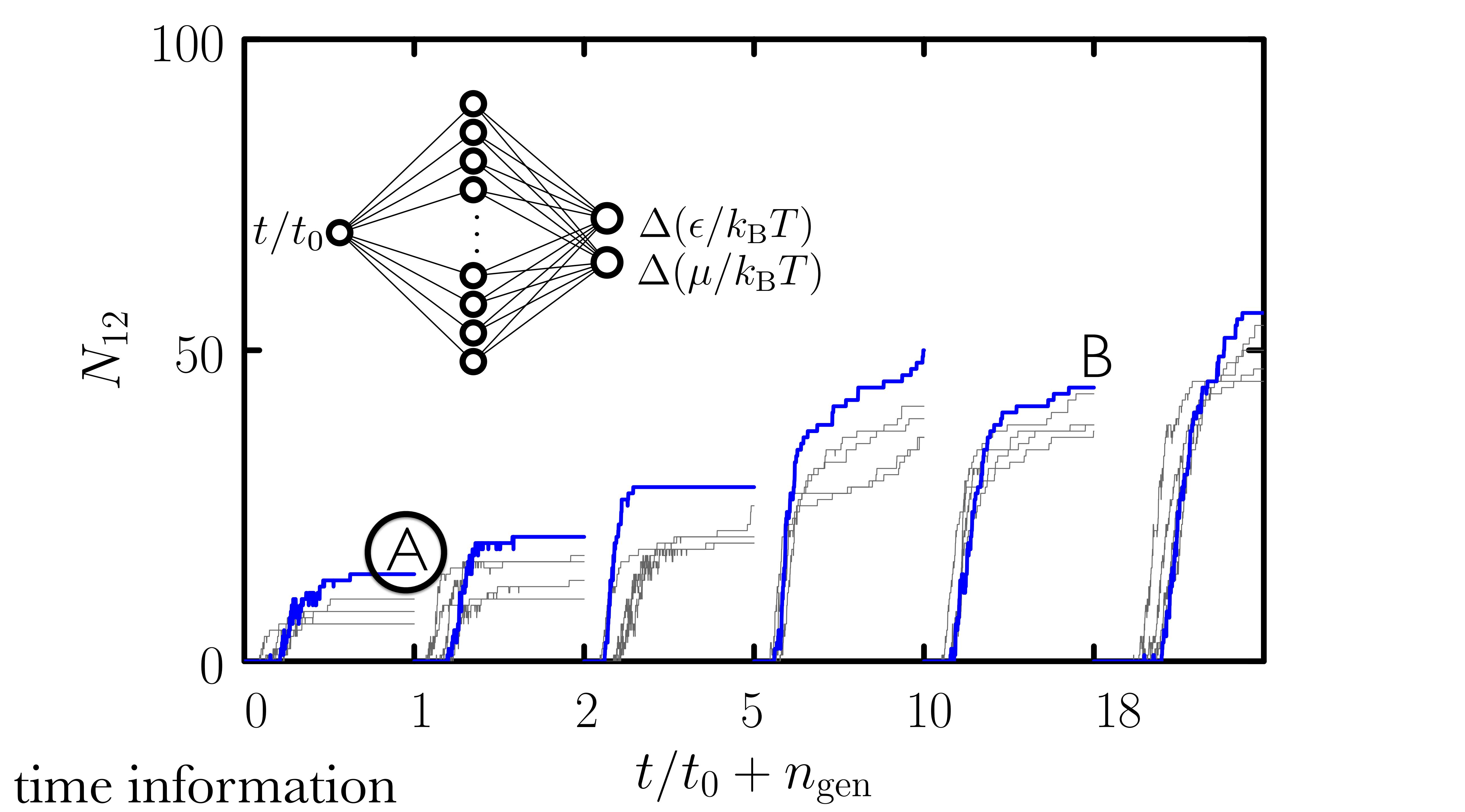
1. HT computational screening of multi-metallic oxides for OER
2. Generative models for surface structure suggestion
3. Synthesis and optimization of catalysts
4. Accelerated testing methods for stability
5. ML platform for material optimization



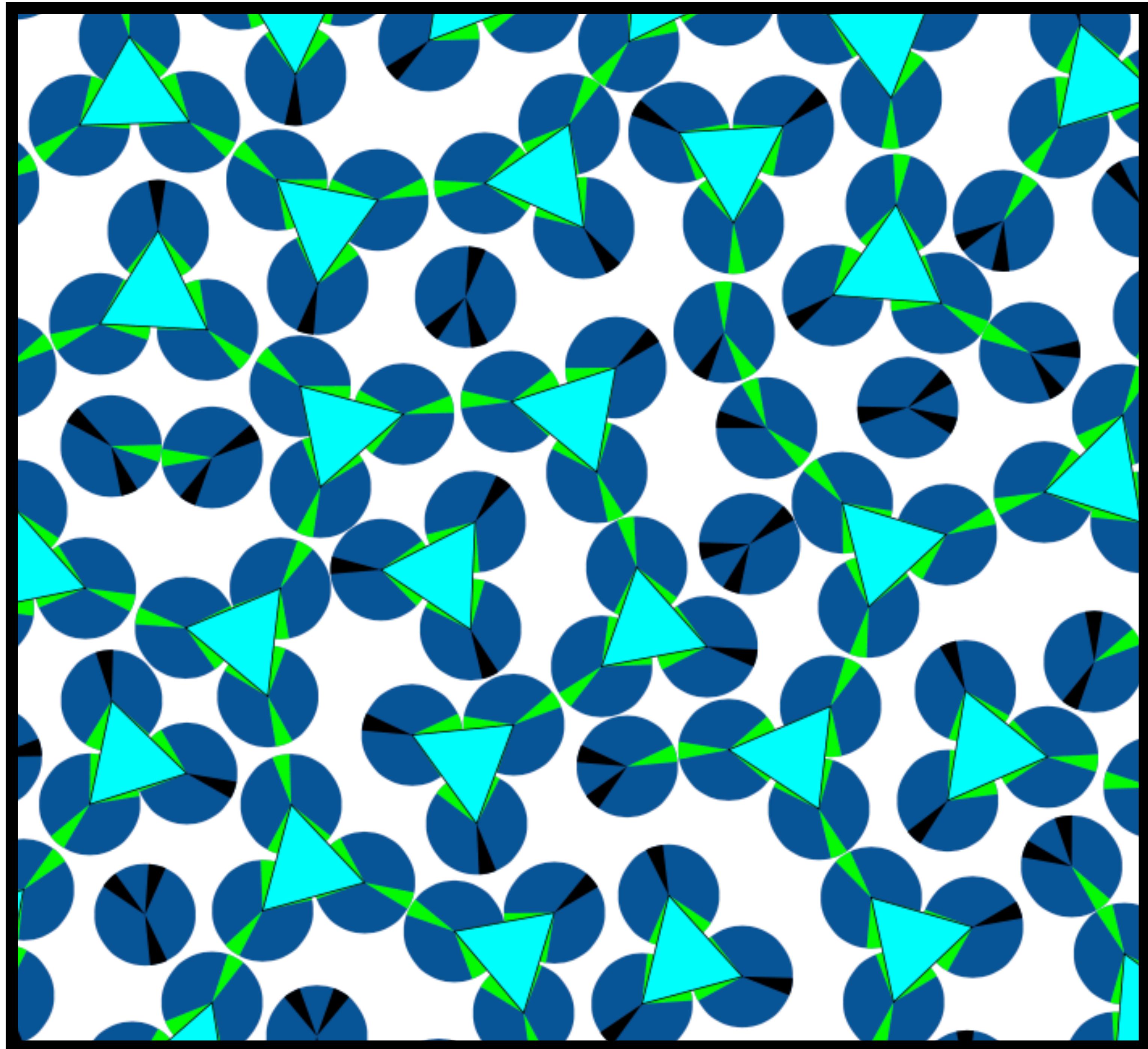


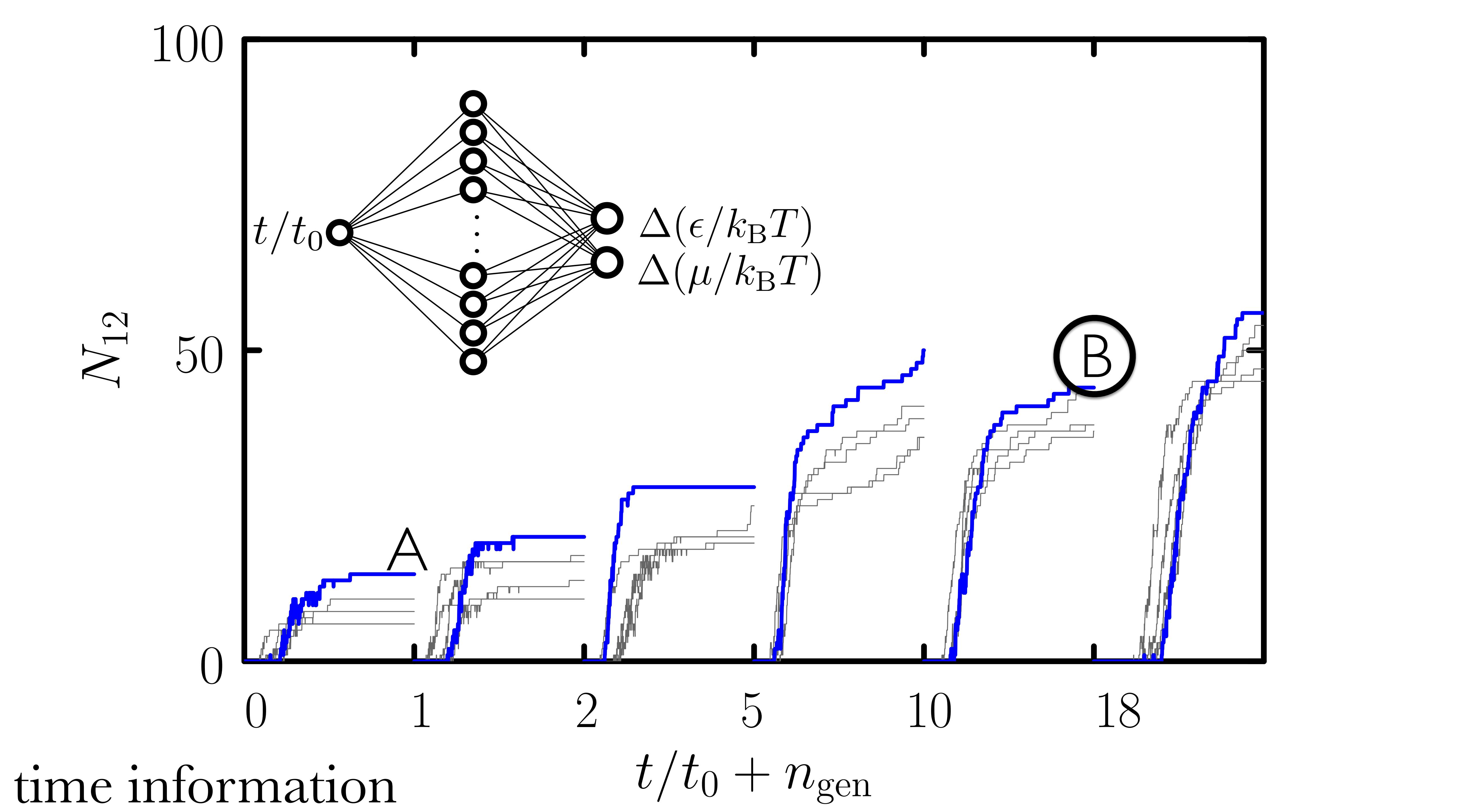
self-assembly kinetic yield networks



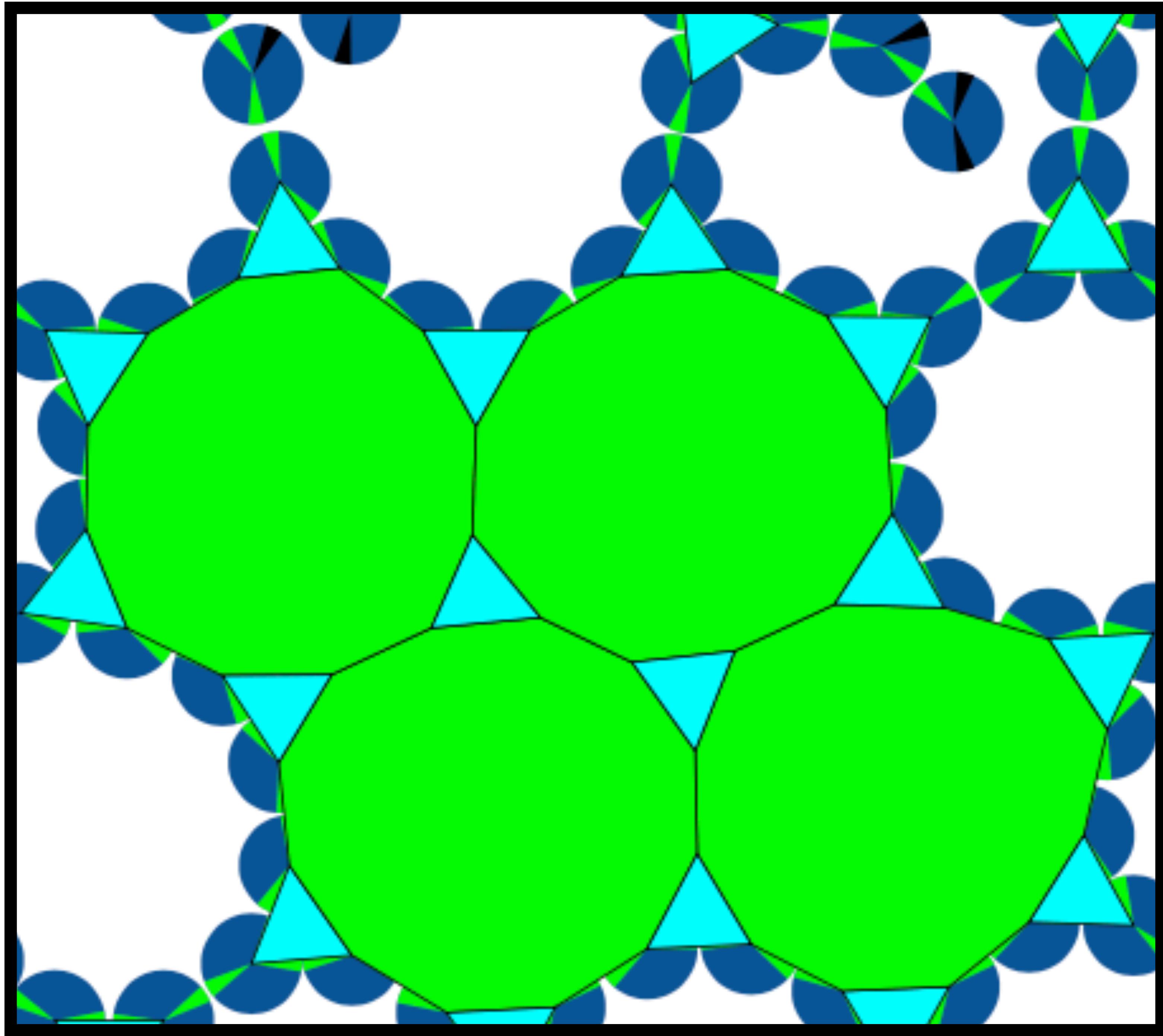


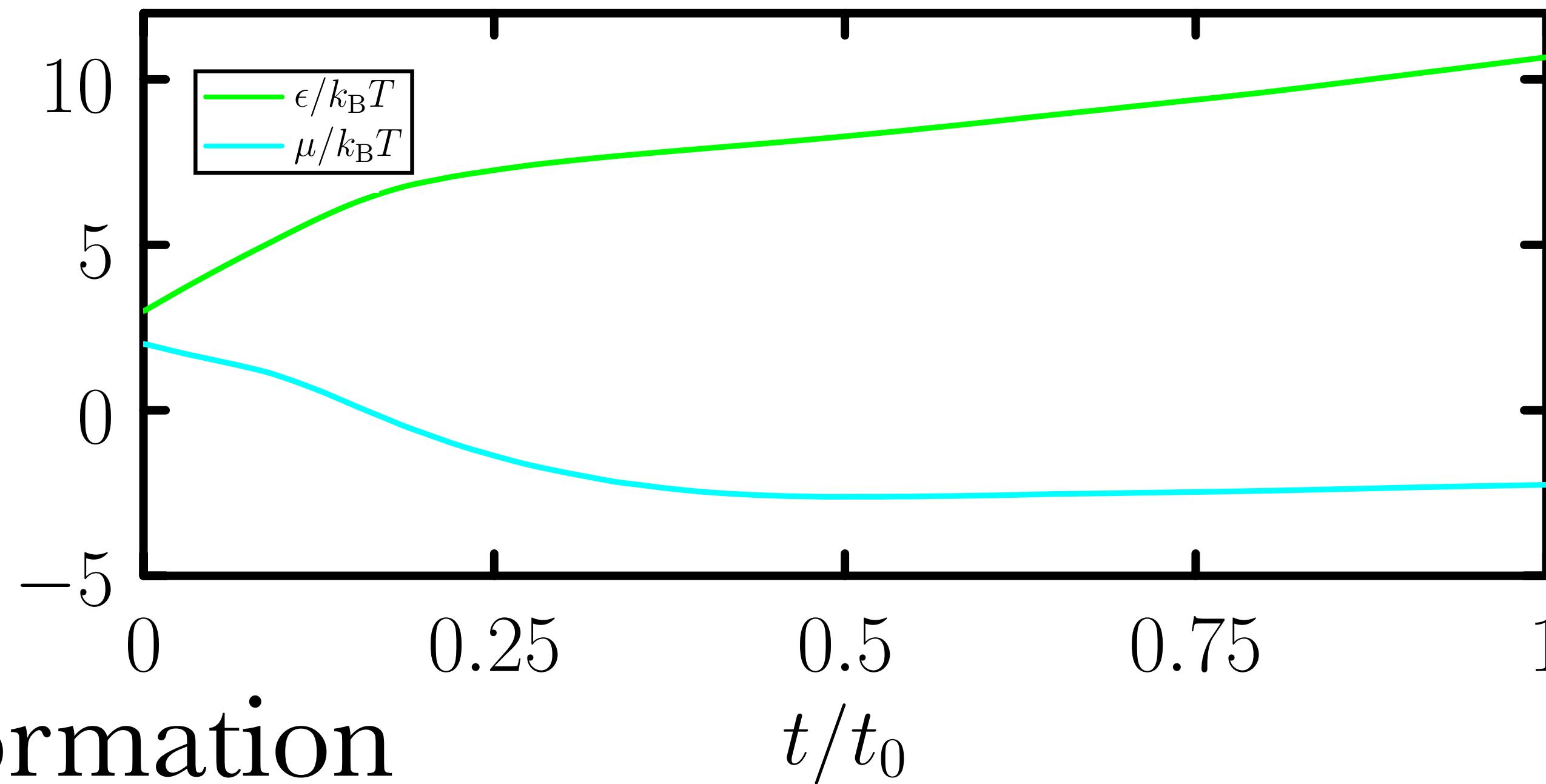
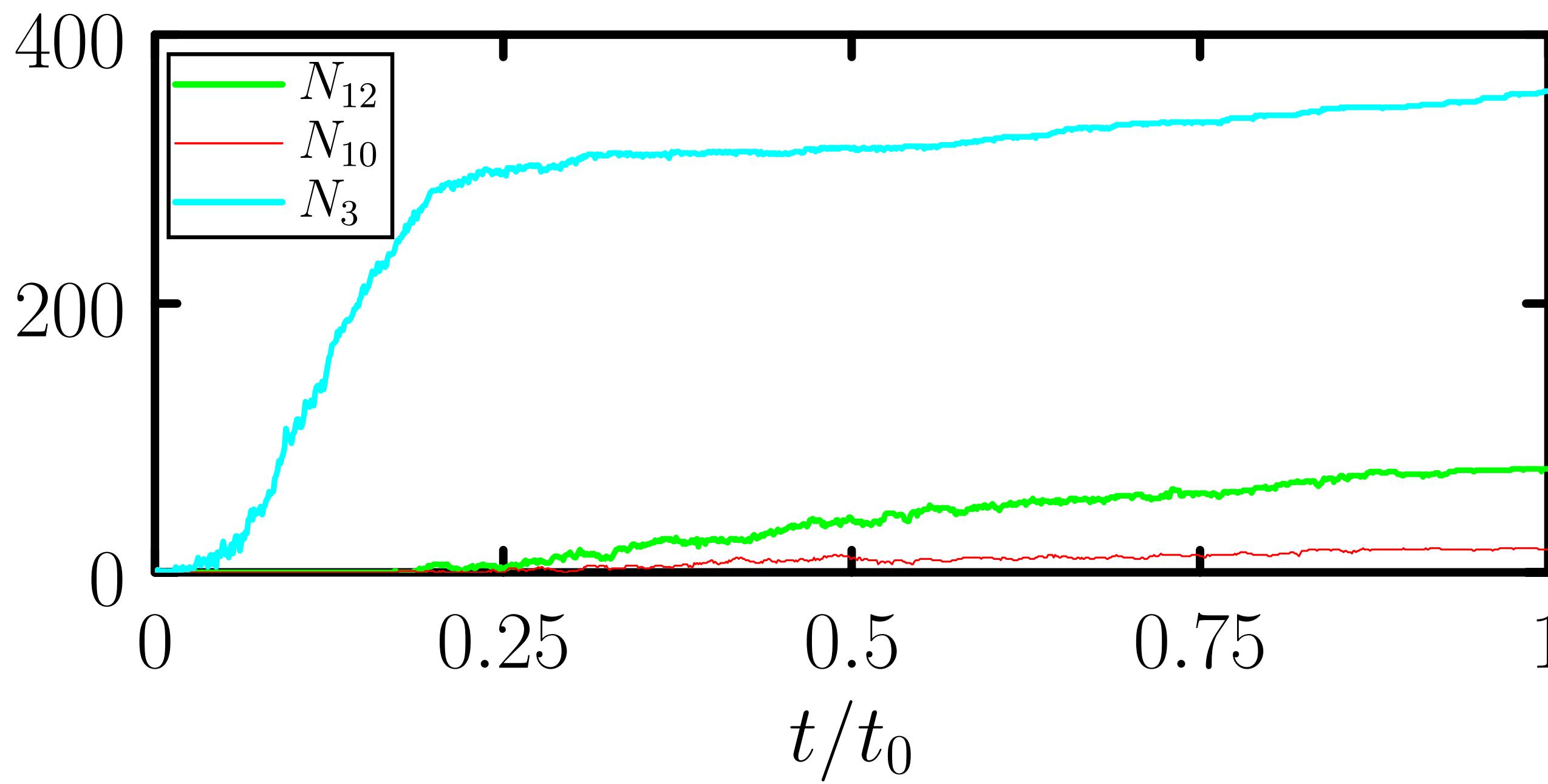
A





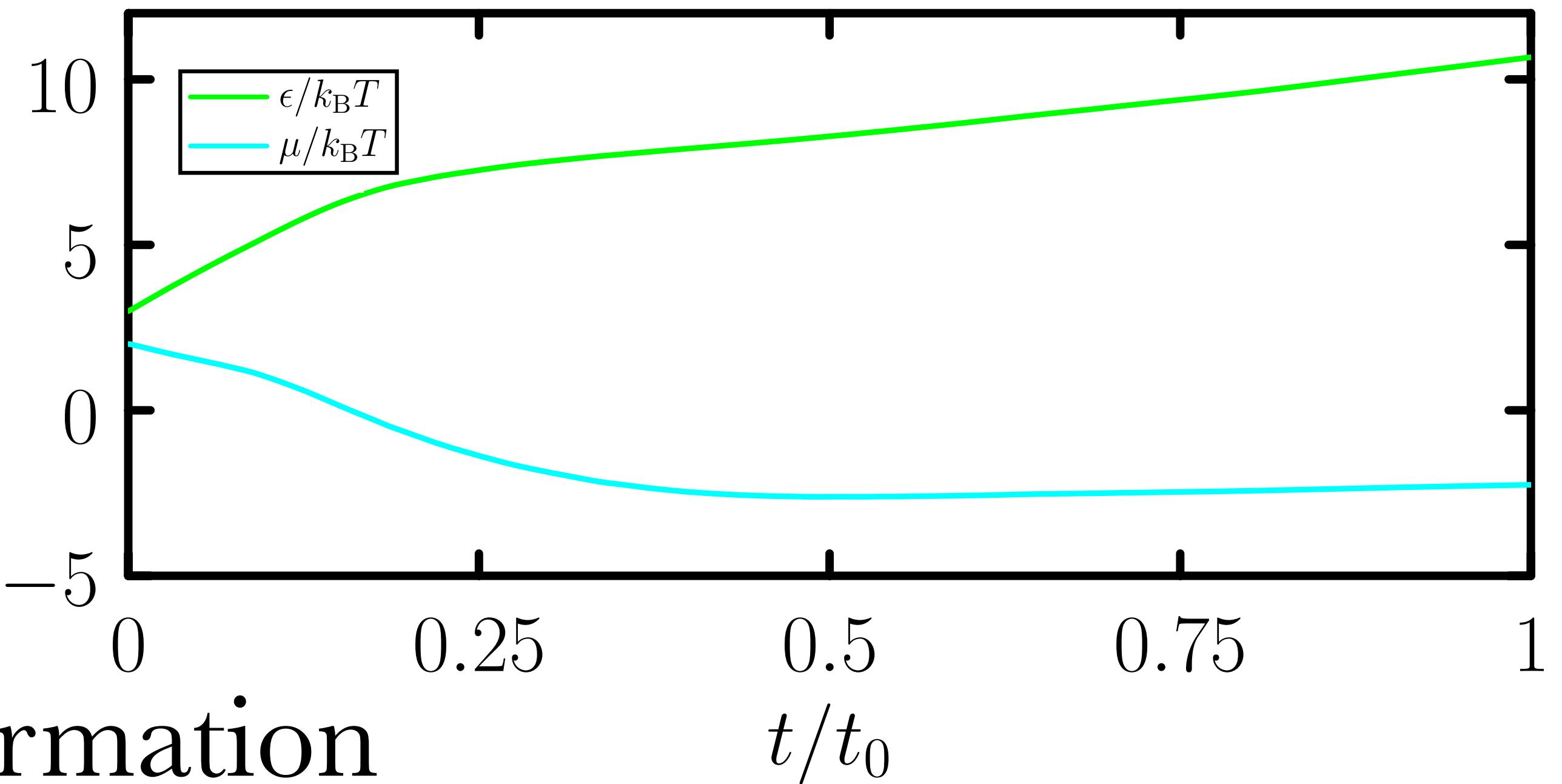
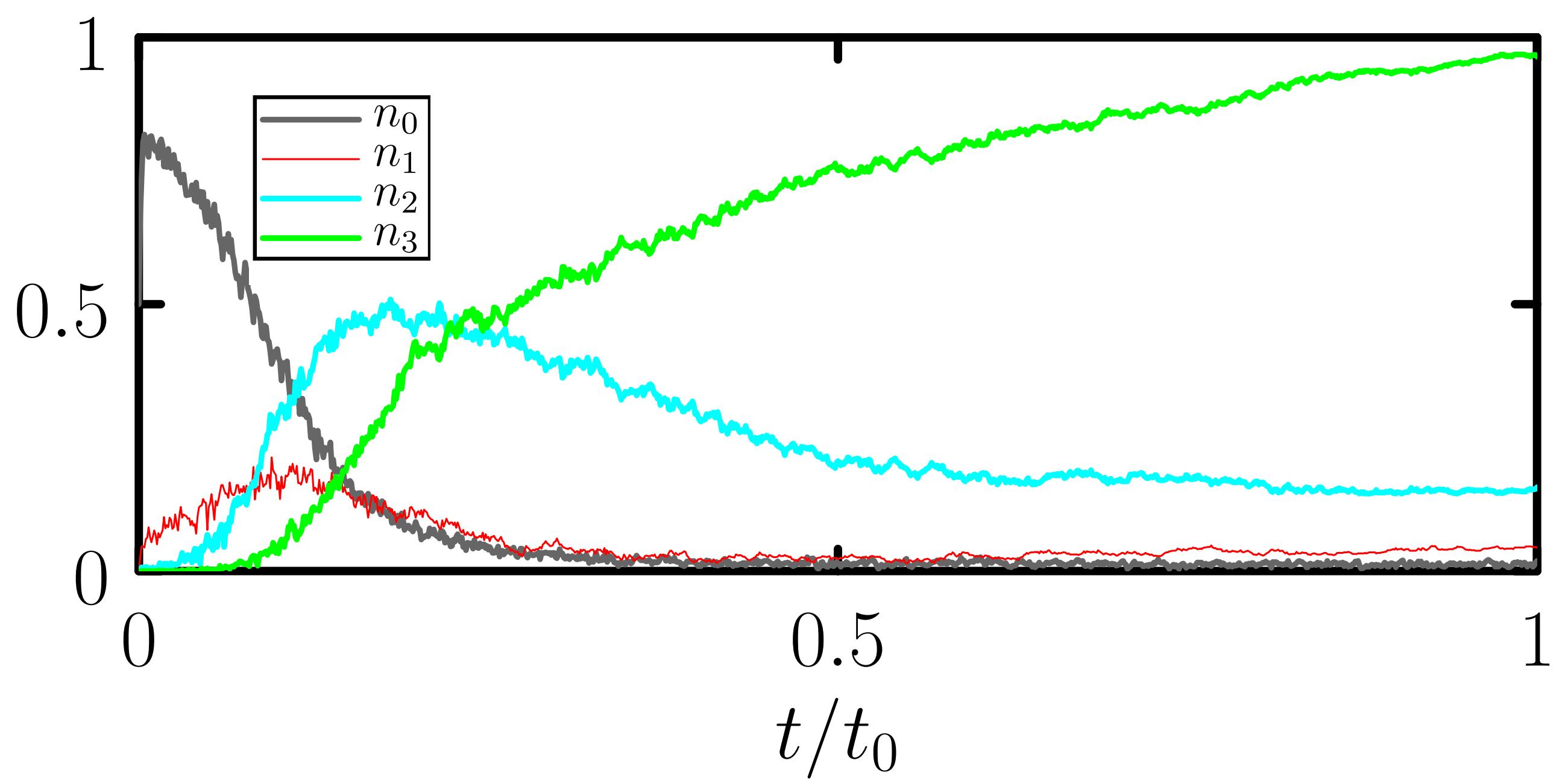
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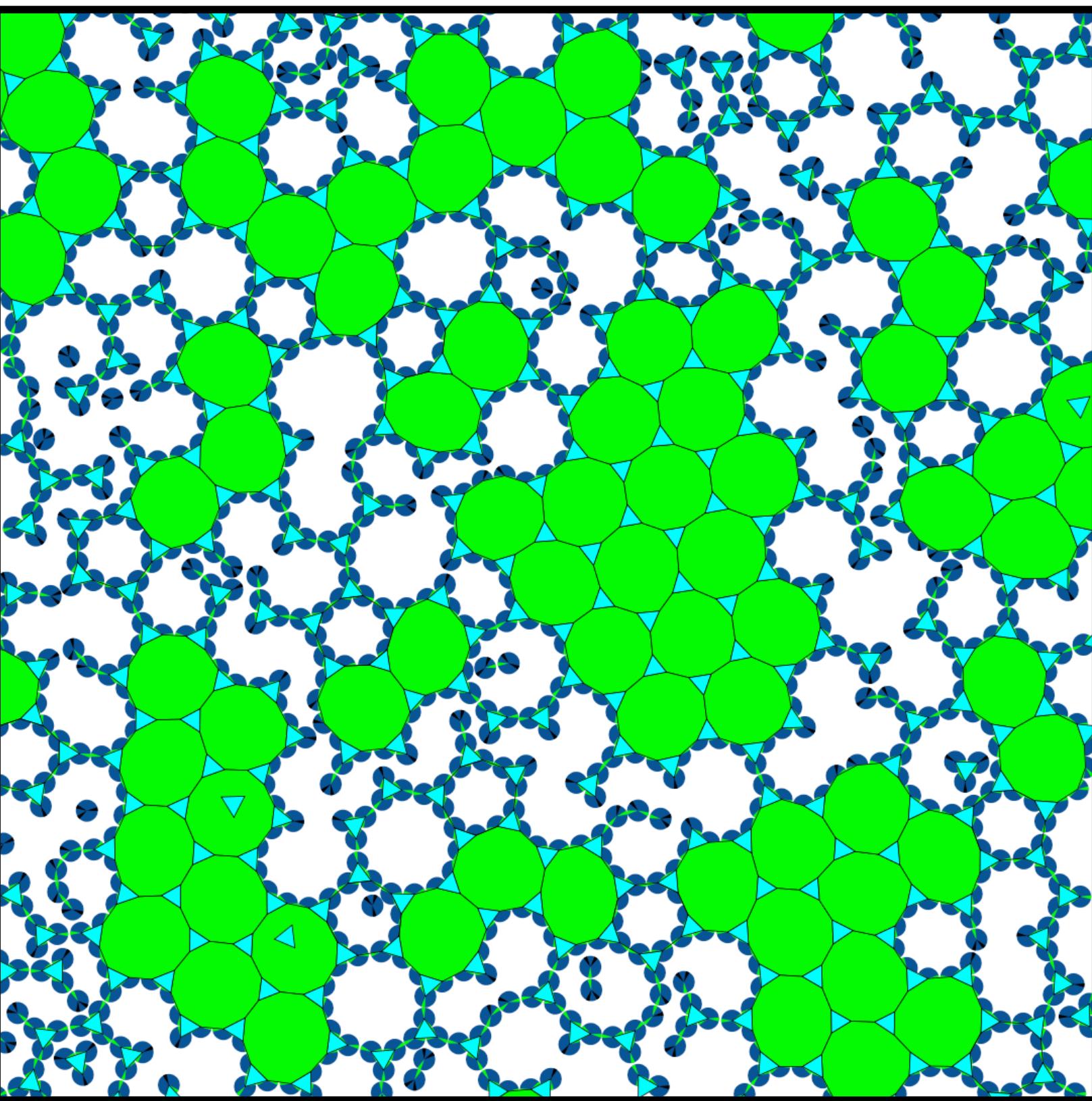
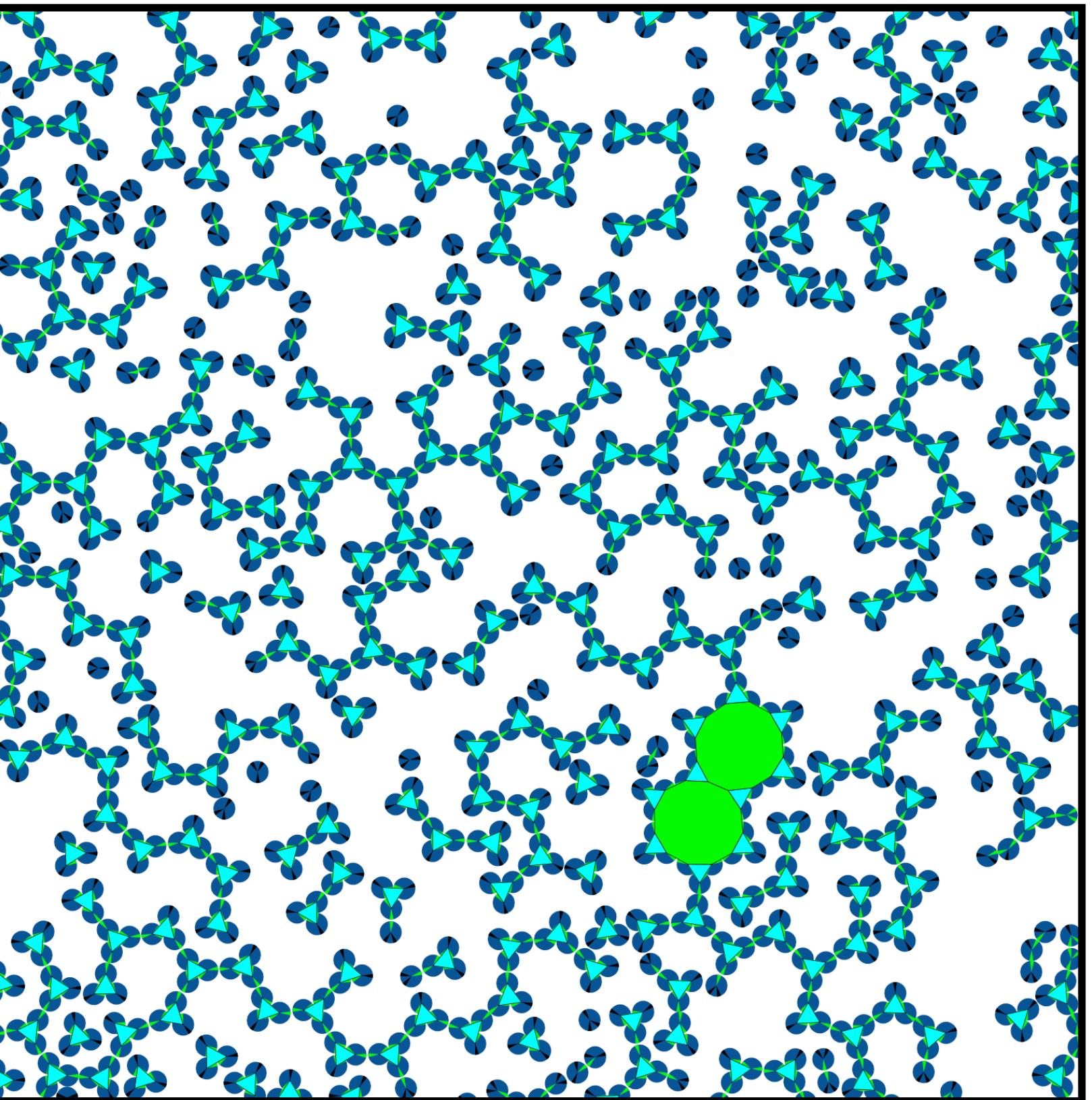
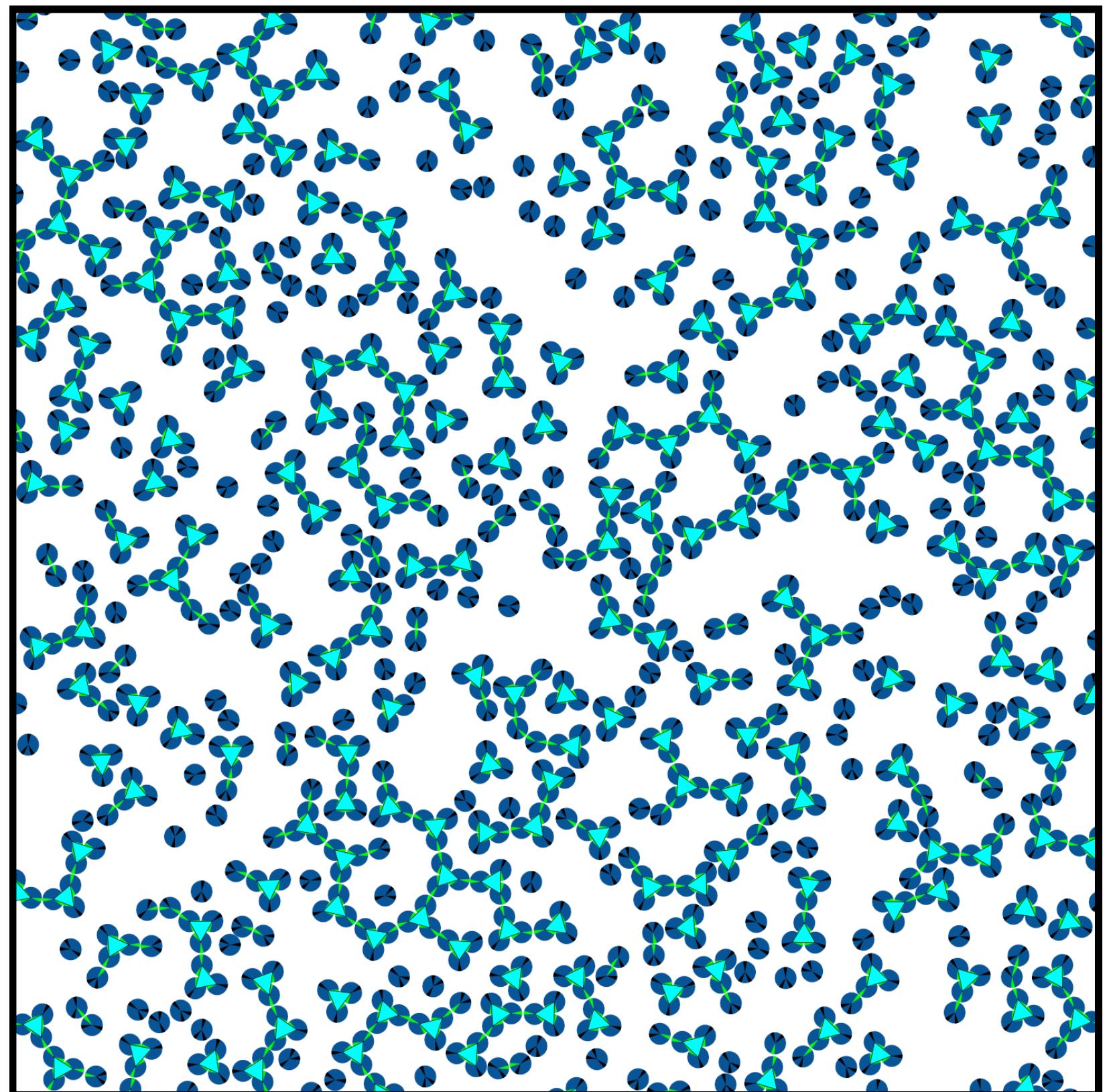
microscopic information

$\pi(\vec{s})$



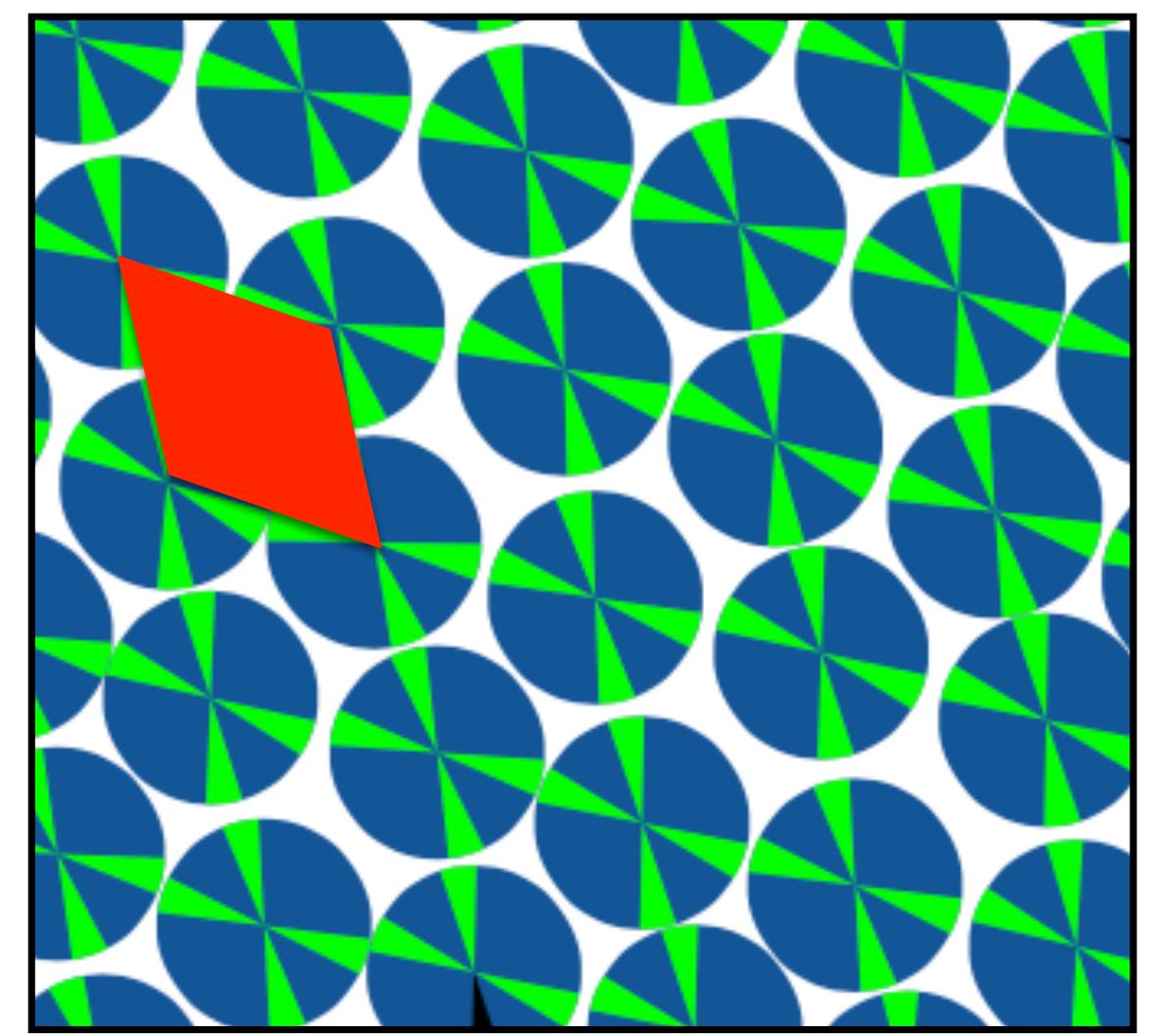
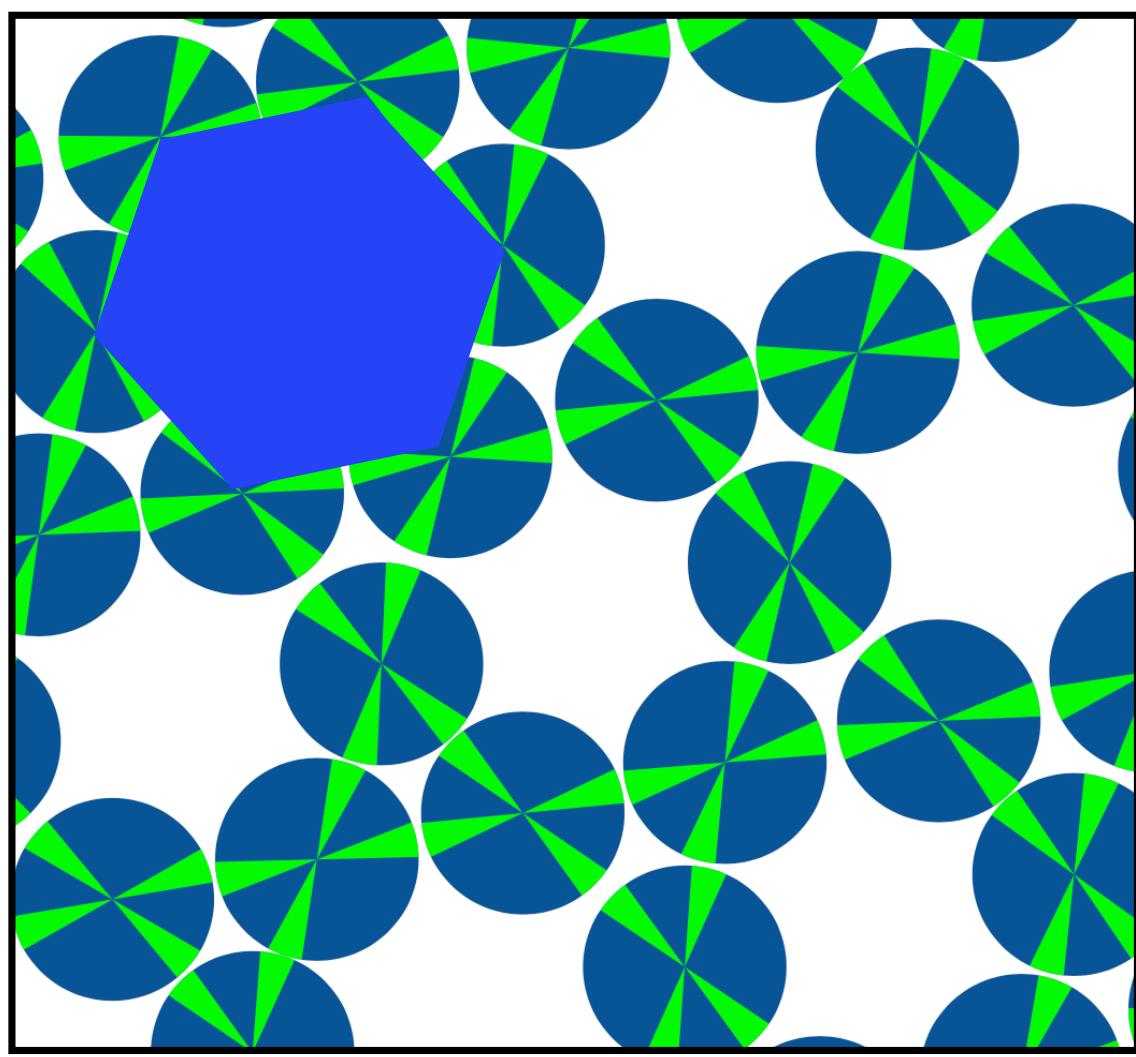
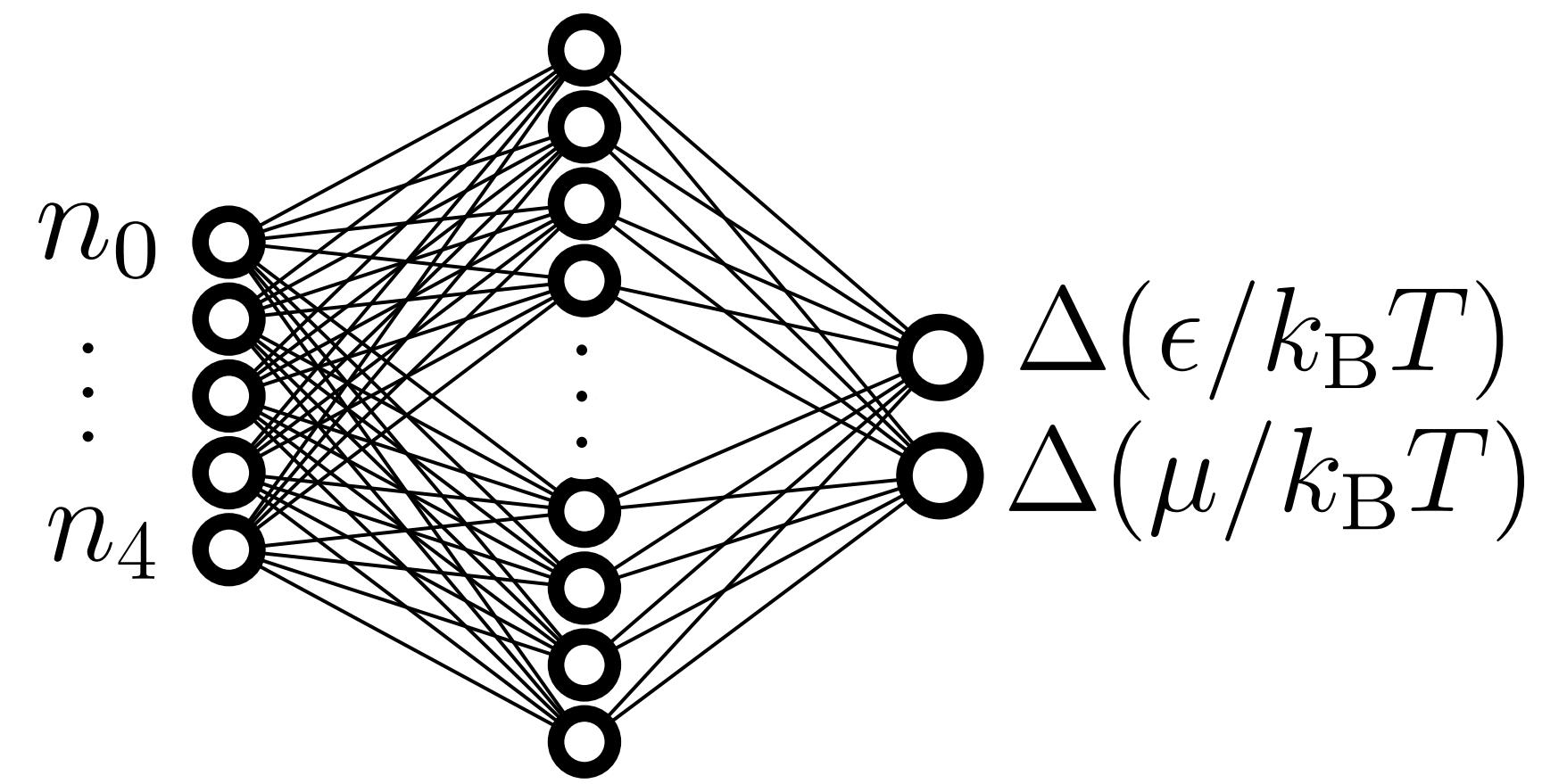
microscopic information

$\pi(\vec{s})$



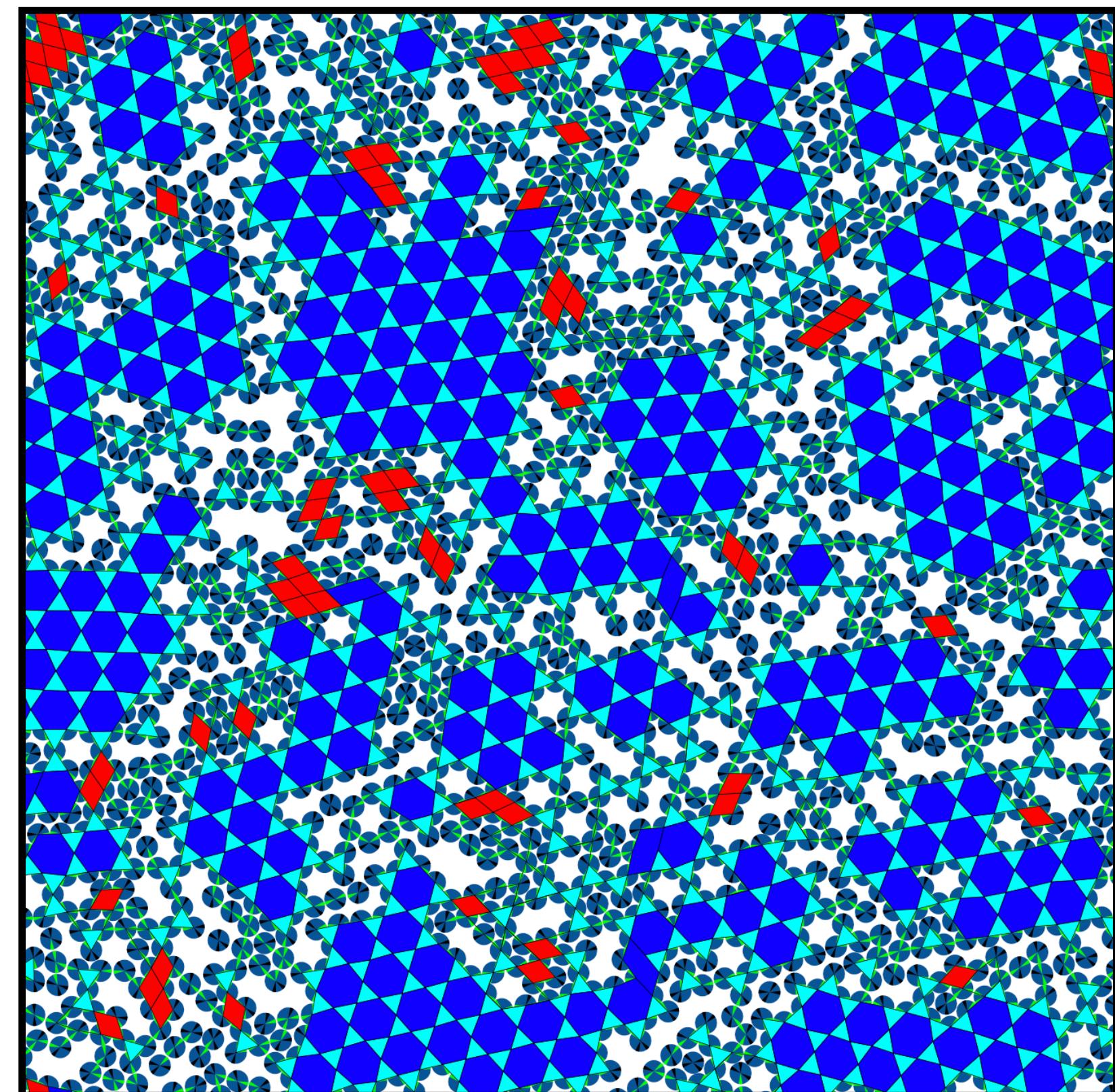
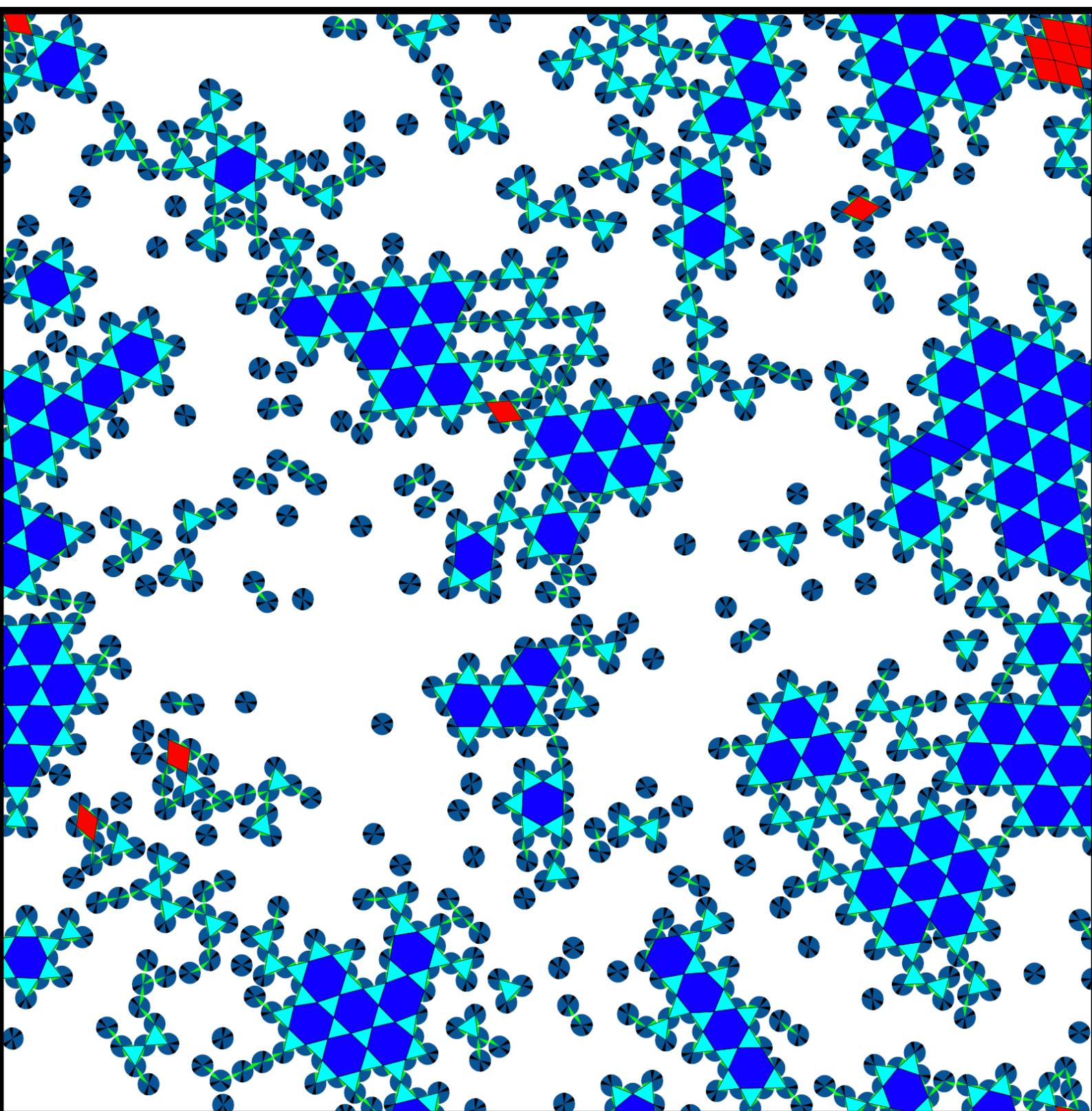
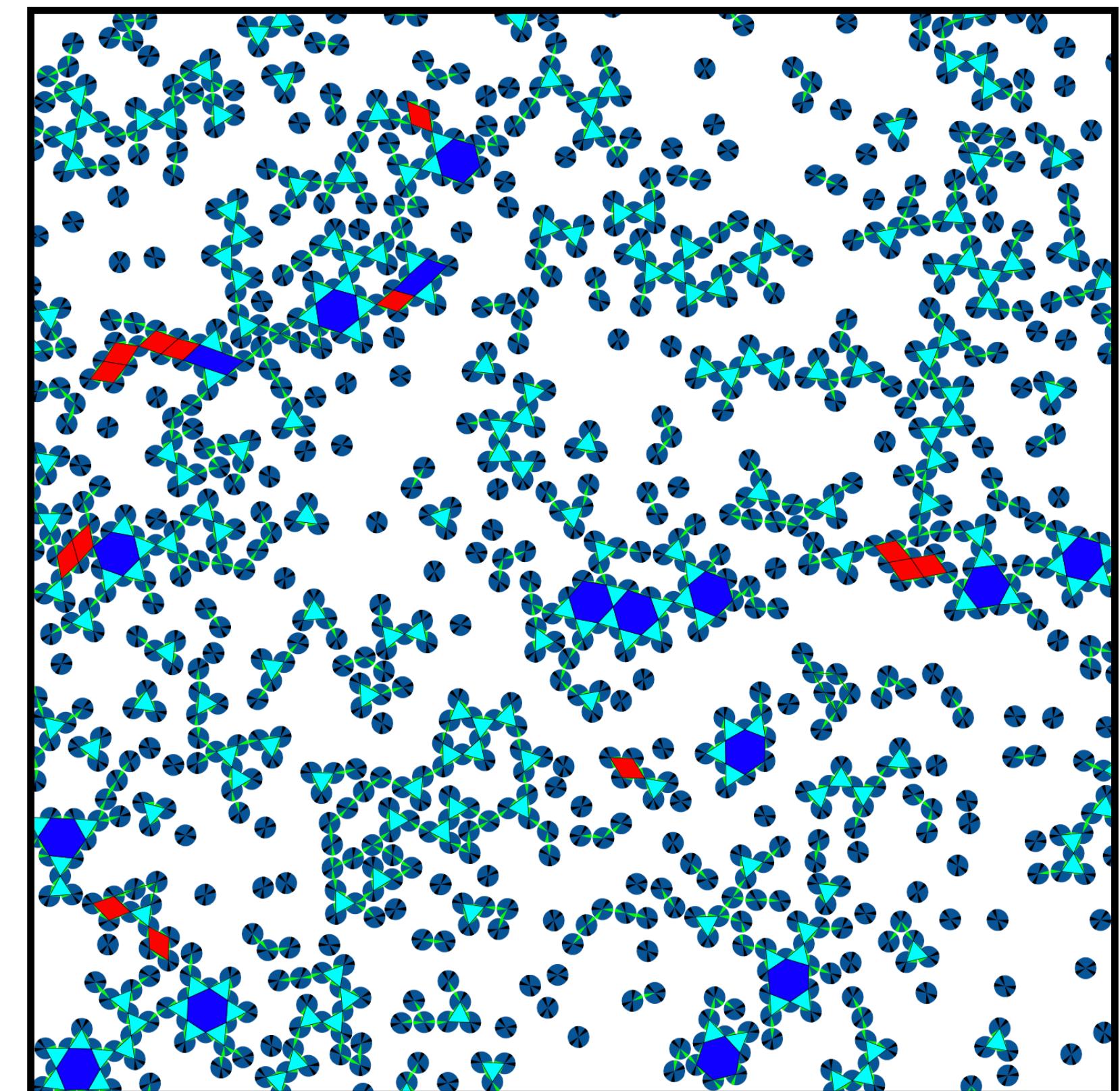
time





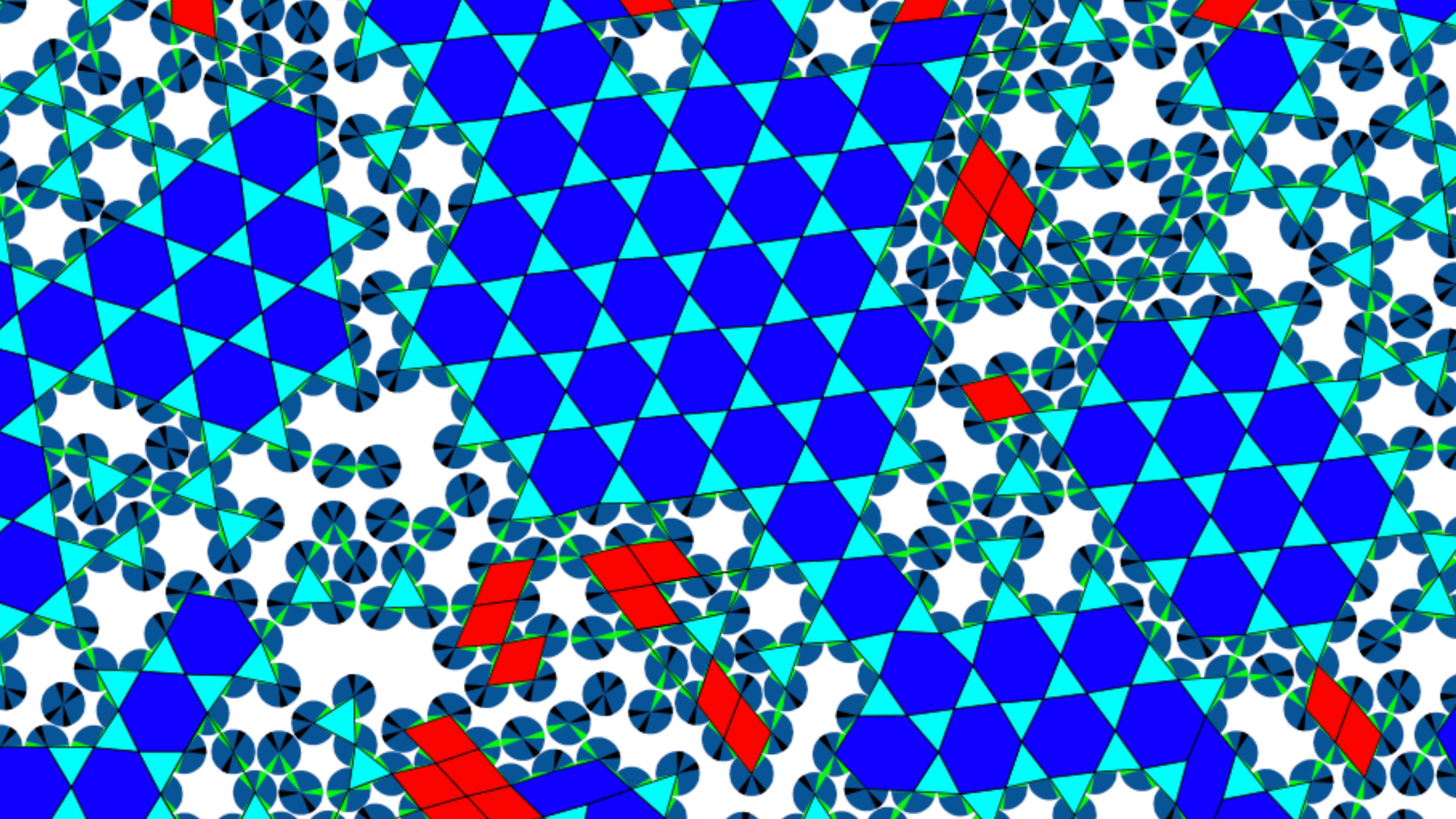
polymorphism

Phase I

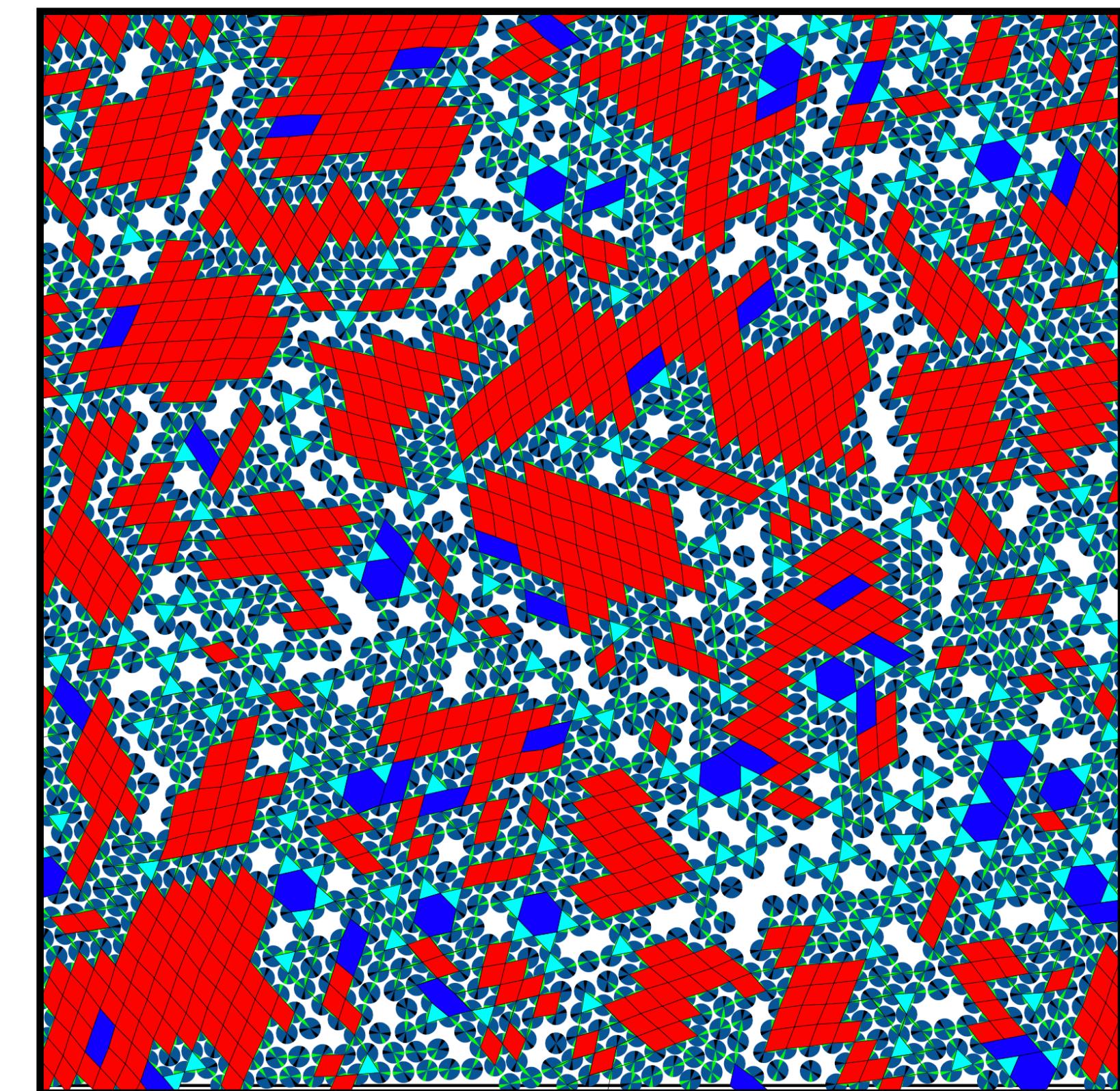
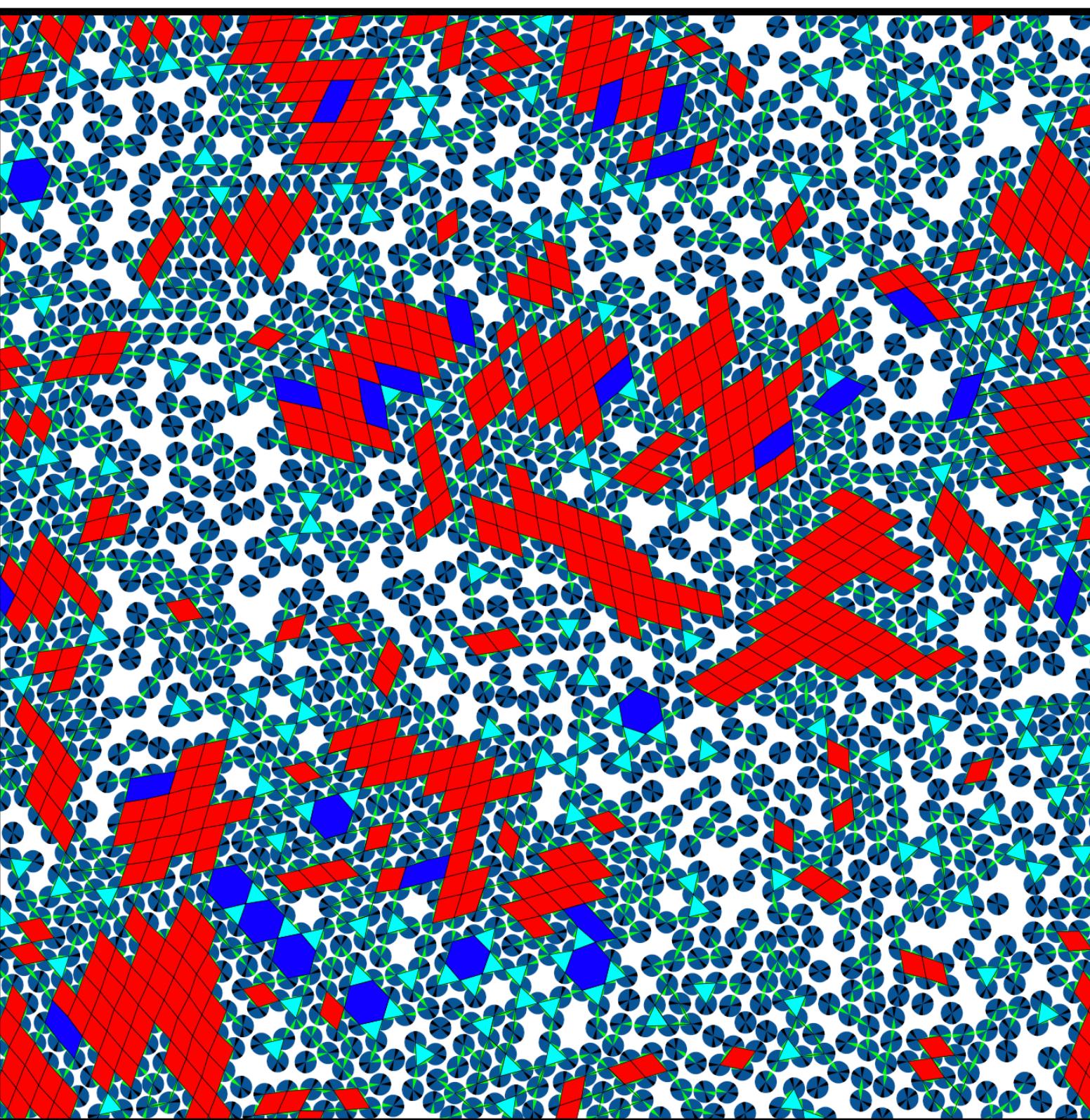
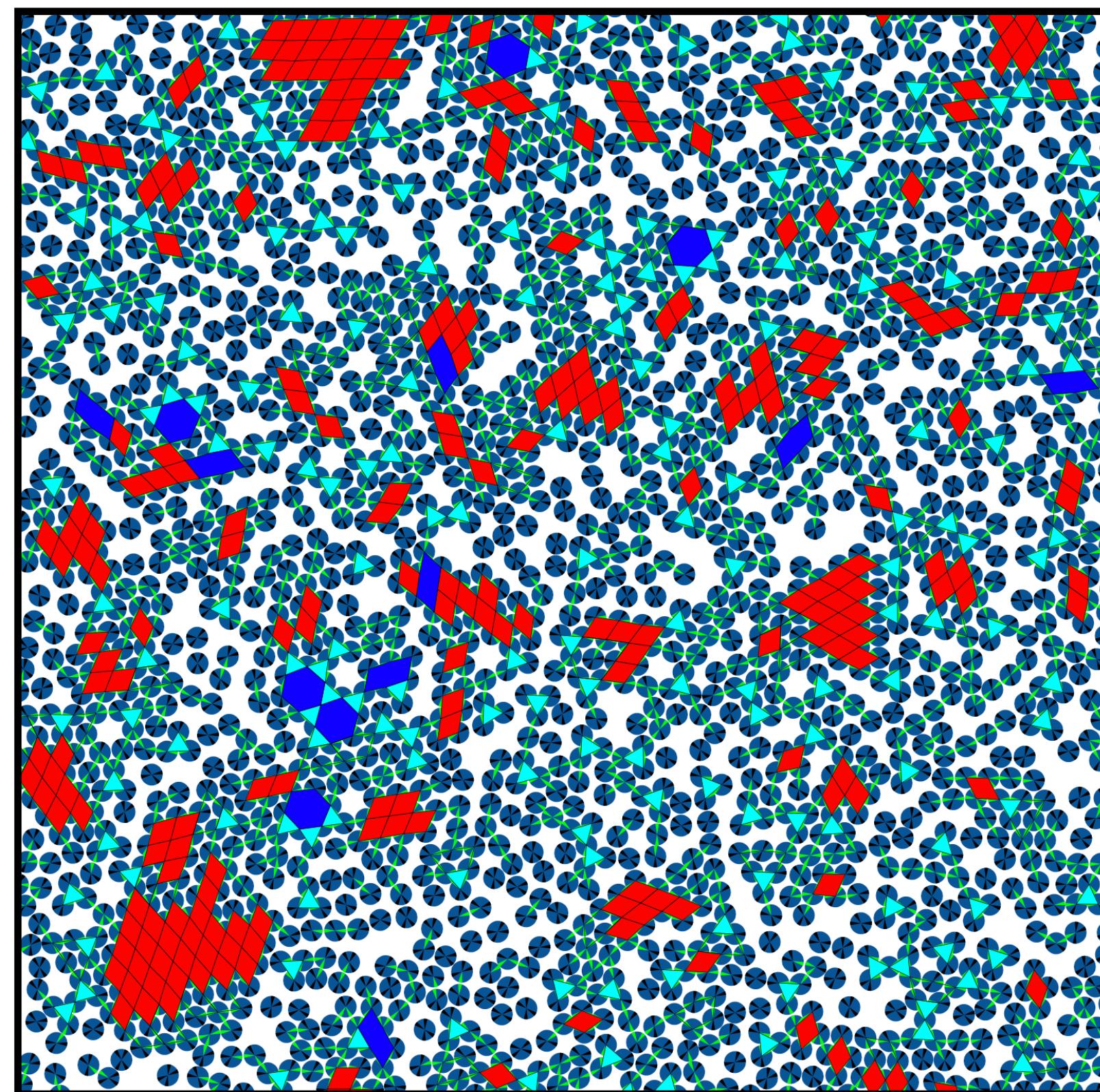


time



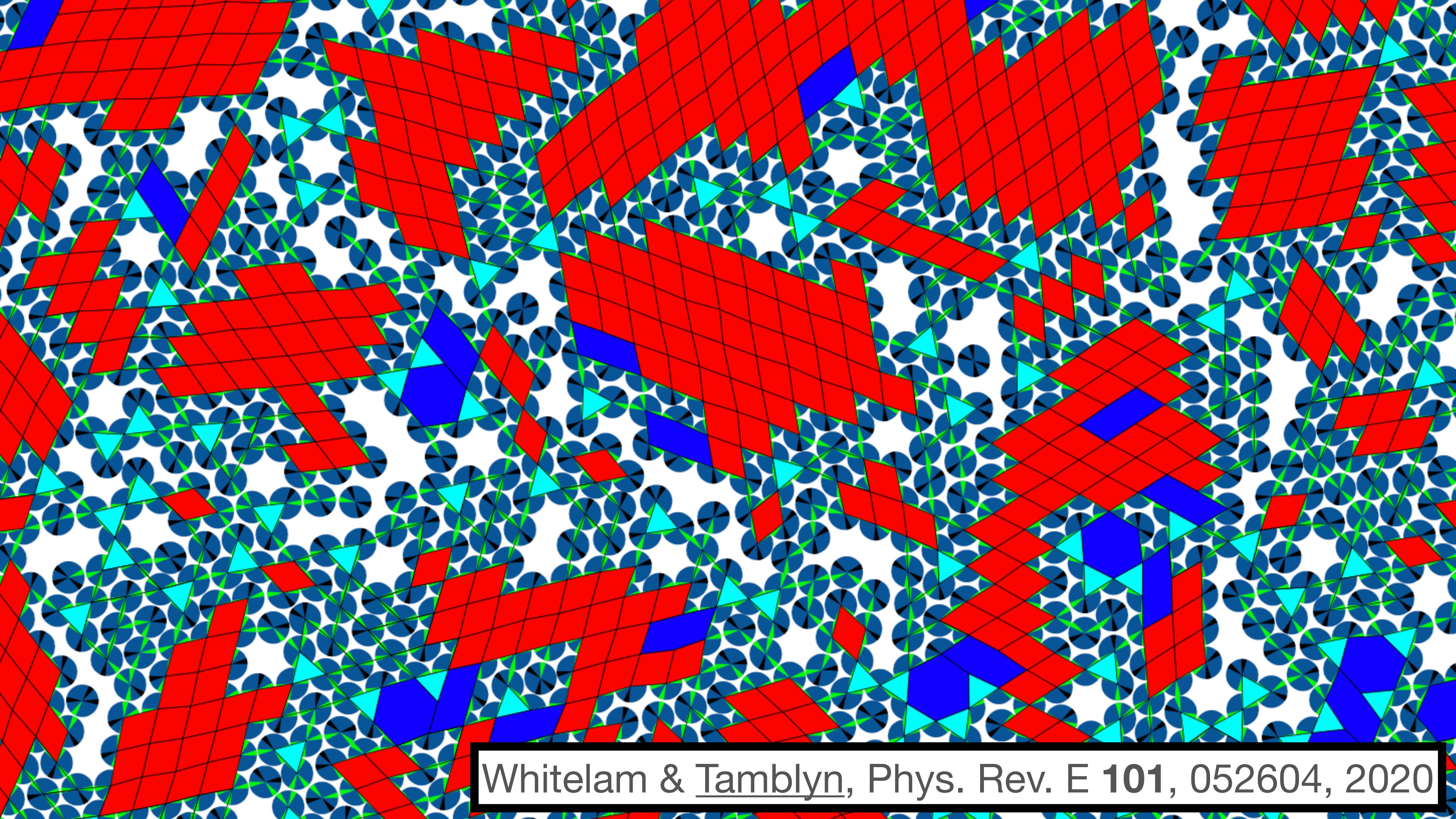


Phase II



time





Whitelam & Tamblyn, Phys. Rev. E 101, 052604, 2020

Thank you!

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