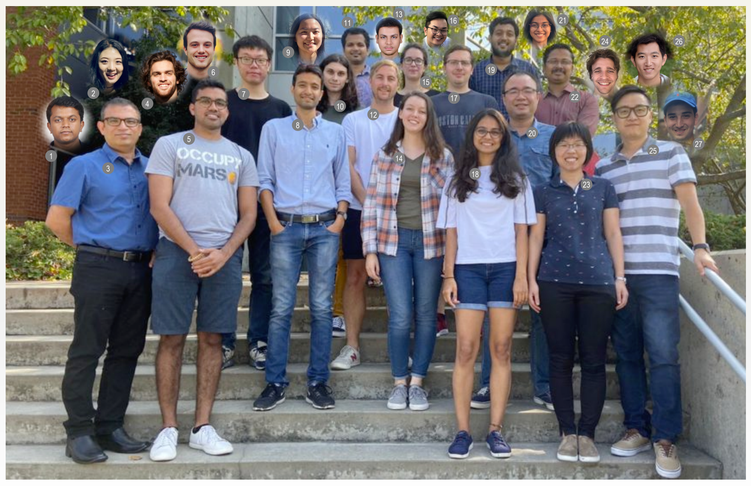
Materials Discovery & Informatics at

RAMPRASAD RESEARCH GROUP

School of Materials Science and Engineering
Georgia Institute of Technology

We develop and utilize computational and data-driven tools to aid materials design



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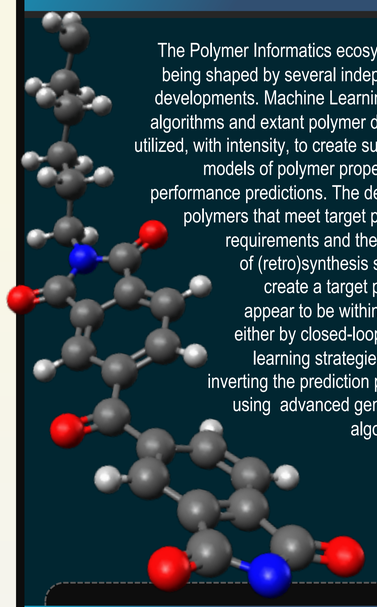
Georgia Institute of Technology · Office of Naval Research · National Science Foundation · US Department of Energy · Toyota Research Institute · Kolon Industries · Exxon Mobil

Polymer Informatics Ecosystem

Khazana - A portal for data and tools from the Ramprasad Research Group

khazana 1.0 — https://khazana.gatech.edu

Data Repository · Polymer Genome · AGNI (DFT Emulator) · ML-Maidan



The Polymer Informatics ecosystem is being shaped by several independent developments. Machine Learning (ML) algorithms and extant polymer data are utilized, with intensity, to create surrogate models of polymer property and performance predictions. The design of polymers that meet target property requirements and the design of (retro)synthesis steps to create a target polymer appear to be within reach, either by closed-loop active learning strategies, or by inverting the prediction pipeline using advanced generative algorithms.

Autonomous Computations

AGNI: ML-Assisted QM Simulations

Semi-Automatic Data Capture

Data integration & management
- Computational data
- Experimental data

Artificial intelligence
- Deep learning, regression, multi-fidelity information-fusion, multi-task learning …
- VAE, genetic algorithm active learning …

Design platform
- New polymers → *Instant property prediction*
- Targeted property → *Accelerated polymer design*

Feedforward new information for adaptive data augmentation

ML-assisted expansion of polymer chemical / property space

Synthesis / Computation
AI-guided & automated data generation
(AI for QM / AI for experiments)

Materials Discovery

Recyclable polymers · *Battery electrolytes* · *Membranes* · *Conducting polymers* · …

Forward Problem

Polymer → *Hierarchical fingerprinting* → *ML prediction model* → ***Instant property prediction***

Inverse Problem

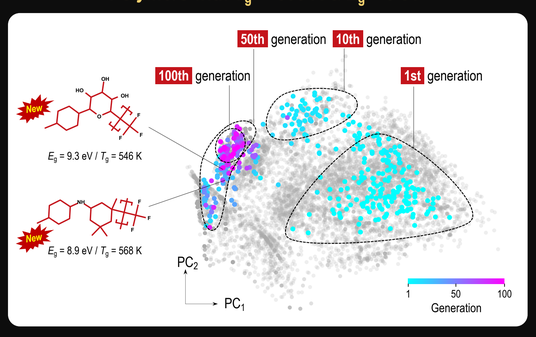
Target property → Variational autoencoder (VAE) / Genetic algorithm / Active learning → ***Polymer designs***

Example discovery
High energy density polymer

New **PDTC-HK511**
Energy density ~16 J/cm³

Reference polymer
BOPP … Energy density ~5 J/cm³

*Example design – using genetic algorithm**
Polymers with T_g^* > 500 K & E_g^* >6 eV



8,453 polymers projected on 2D principal component (PC) space (PC generated using the polymer fingerprints). All polymers created during 100 generations are represented by gray points. Area of polymers created at the generation #1, 10, 50, and 100 are selected to visualize the convergence in chemical diversity with evolution.

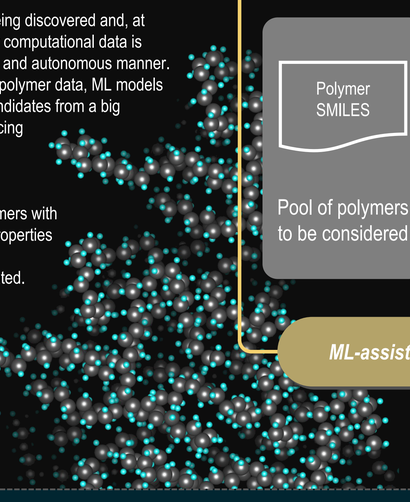
**Genetic algorithm* … A powerful method for solving materials design problems based on natural selection, the process that drives biological evolution.
*T_g … glass transition temperature), E_g … bandgap

- Polymer design using genetic algorithm and machine learning (Comput. Mater. Sci., 186, 110067, 2021)
- Polymers for extreme conditions designed using syntax-directed variational autoencoders (Chem. Mater. 32, 10489, 2020)
- Active-learning and materials design: the example of high glass transition temperature polymers (MRS Comm 9, 860, 2019)
- Rational co-design of polymer dielectrics for energy storage (Advanced Materials, 28, 6277, 2016)

Autonomous Computations

ML-guided design of computations (and experiments) expands and diversifies the polymer data.

Functional polymers are being discovered and, at the same time, high-quality computational data is being created in a targeted and autonomous manner. Starting from the available polymer data, ML models are developed to select candidates from a big dataset of polymers, balancing between exploitation and exploration. 3D models of the candidates are then predicted, from which polymers with targeted (computational) properties are identified and data are progressively curated/updated. Requiring minimal human intervention, this autonomous workflow will be the primary source of computational data for polymers informatics.



Polymer data → *ML surrogate model* → *SMILES to 3D structure generator*

Polymer SMILES → Pool of polymers to be considered → Select polymers for the next calculation → Polymer ■ / Polymer ▲ / Polymer ● / Polymer ◆ → High-throughput computation → ***ML-assisted expansion of polymer chemical / property space***

- A multi-fidelity information-fusion approach to machine learn and predict polymer bandgap (Comput. Mater. Sci., 172, 109286, 2019)

Polymer Genome

www.polymergenome.org

User input
SMILES, name, abbreviation, sketch

General information
Polymer class, IUPAC name, similar polymers

"A Machine Learning Platform for New Polymer Discovery"

Predicted properties Polymer properties predicted by ML models

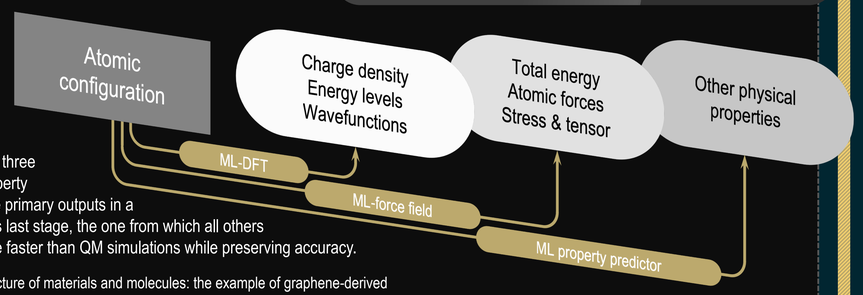
- Electronic properties - Bandgap, ionization energy, electron affinity
- Dielectric & optical properties - Dielectric constant, refractive index
- Thermal properties - Glass transition Temp., melting temp., thermal decomposition Temp.
- Solubility properties - Solvent & non-solvent, solubility parameter
- Permeability properties - Gas permeability, selectivity
- Mechanical properties - Tensile strength, Young's modulus
- Physical & thermodynamic properties - Density, atomization energy, specific heat
- Other properties - Tendency to crystalize, limiting oxygen index
- Structure - 2D & 3D structure of monomer

- Polymer Genome: a data-powered polymer informatics platform for property predictions (J. Phys. Chem. C 122, 31, 17575-17585, 2018)
- Machine-learning predictions of polymer properties with Polymer Genome (J. Appl. Phys., 128, 171104, 2020)

Structure visualizer
3D structure of monomer, 'mol' file

AGNI: ML-Assisted QM Simulations

Deep learning based-QM simulations can be performed at three stages, each with a different objective in mind: 1) as a property predictor; 2) as a force-field generator; and 3) to obtain the primary outputs in a DFT calculation, namely the charge density and DOS. This last stage, the one from which all others can be reached (or derived) is several orders of magnitude faster than QM simulations while preserving accuracy.

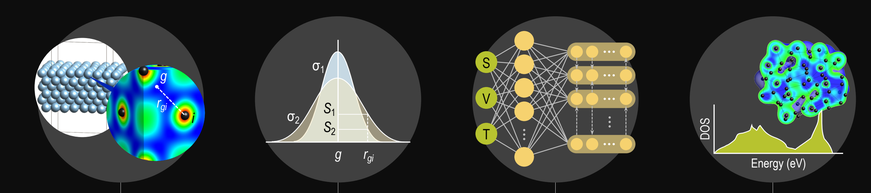


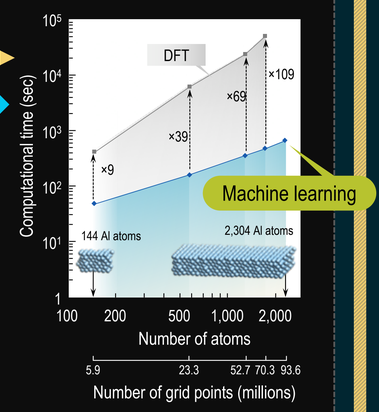
- An efficient deep learning scheme to predict the electronic structure of materials and molecules: the example of graphene-derived allotropes (J. Phys. Chem. A, 124, 9496, 2020)
- Solving the electronic structure problem with machine learning (npj Comput. Mat. 5, 22, 2019)
- General atomic neighborhood fingerprint for machine learning based methods (J. Phys. Chem. C 123, 15859, 2019)
- A universal strategy for the creation of machine learning-based atomistic force fields (npj Comput. Mat. 3, 27, 2017)
- Learning scheme to predict atomic forces and accelerate materials simulations (Phys. Rev. B 92, 094306, 2015)

Ultrafast DFT emulation

Computational time & scaling ▶

Step 1 … Data generation → *Step 2 … Fingerprinting* → *Step 3 … Machine learning* → *Step 4 … Validation*





Semi-Automatic Data Capture

Natural language processing (NLP) enables automated extraction of information & data curation. Most polymer domain knowledge like polymer properties and synthesis recipes are locked up in journal papers in plain text, tables and figures. The goal is to convert this information into machine readable databases or represent it in a high dimensional latent space to capture the information in the continuously growing polymer literature. ML models can then be built on top of this to predict properties and perform polymer design.

Polymer data

Collect Information

Available data sources: doi · ELSEVIER · WILEY Publishers Since 1807 · Crossref

Polymer specific records → Collect papers

Data Capture

- Text containing property information
- Parsing HTML/XML documents and tokenizing
- Tabular information
- Synthesis containing paragraphs

Natural language processing (NLP)

… Poly(ethylene oxide) powder was studied using STM … → Neural network: Train word vectors → New knowledge gained

Tokenized text

Text parsing & computer vision