Towards Machine-driven Discovery of Organic Materials

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Research Computing and Data Seminar Series Spring 2024

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Our team

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Camron De'vine (Undergraduate)
Maxwell Duff (Undergraduate)
Corrine Elliott (Undergraduate)
Tristan Finn (Undergraduate)
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Corey Roberts (Undergraduate)
Andrew Smith (Undergraduate)
William Allen Smith (Undergraduate)
Mitchell Stokan (Undergraduate)
Parker Sornberger (Undergraduate)
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Brandyn Thompson (Undergraduate)
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Ally Watrous (High School)

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Award No. 1627428
Cooperative Agreement No. 2019574

Arnold and Mabel Beckman Foundation

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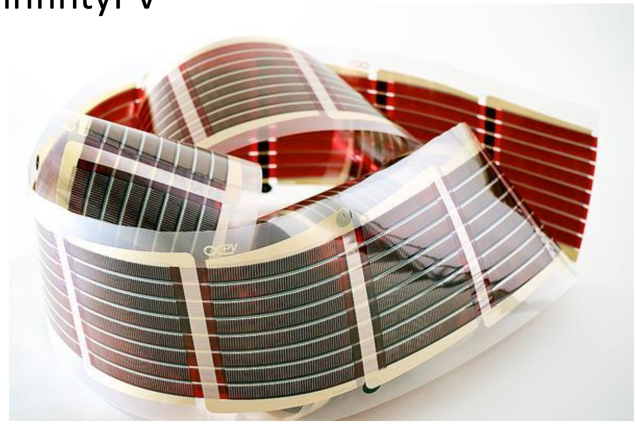
Organic semiconductors

Samsung

University of Tokyo

LG

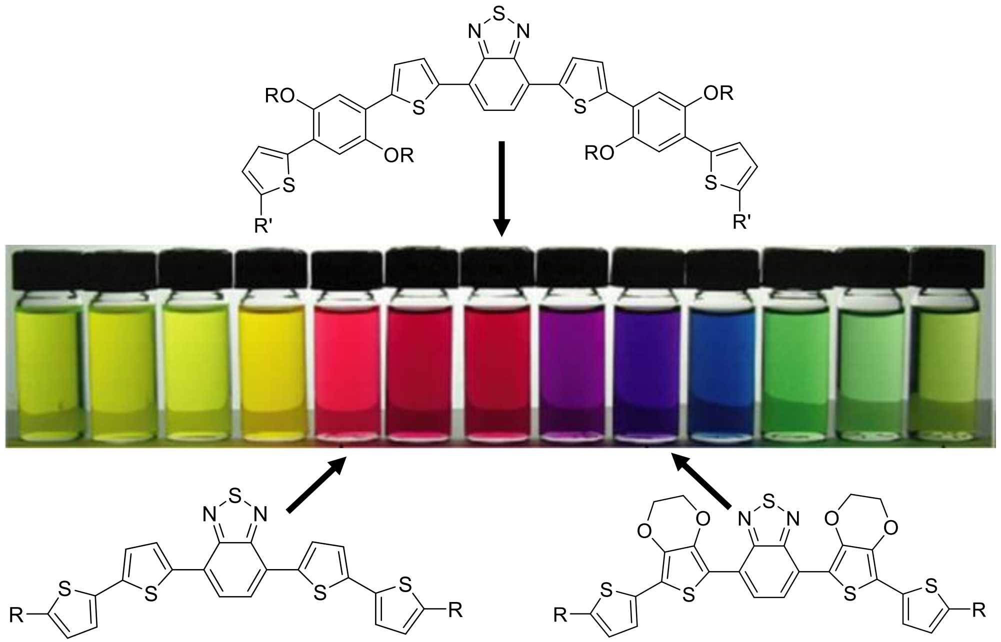
infintyPV



LG

Why organic semiconductors?

- Chemical versatility
  - The power of synthetic chemistry to control redox and optical properties
- Synthetic materials (not mined) that can be (current research) made from bio feedstocks and biodegradable



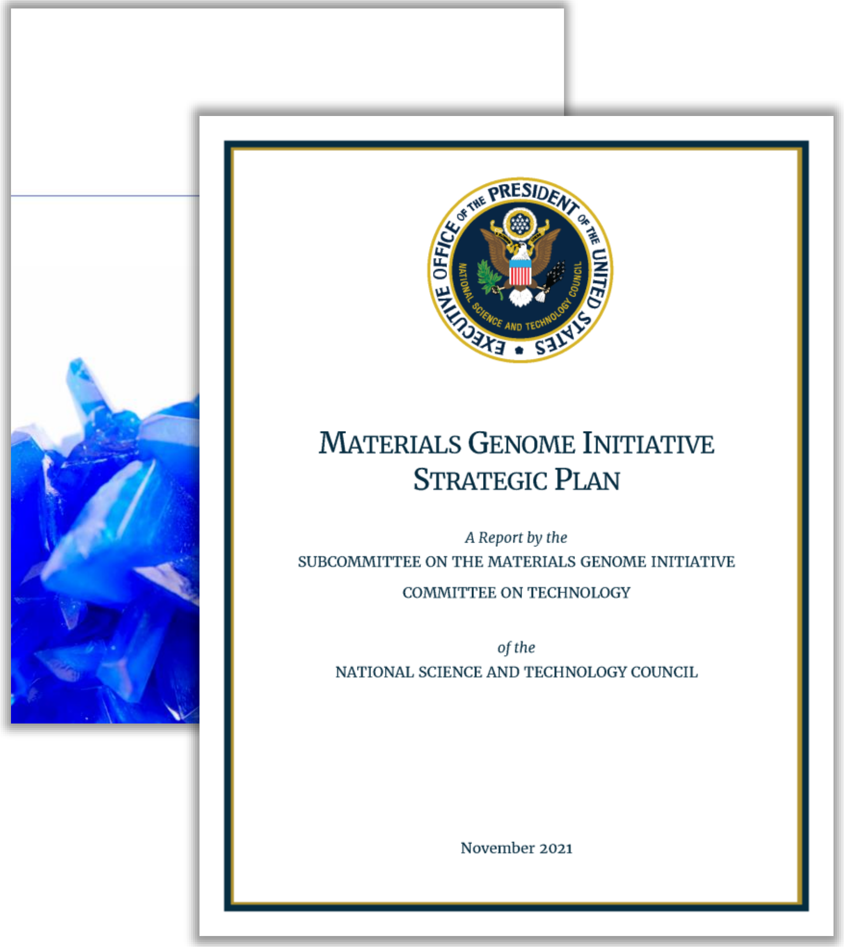
Discrete oligomers / Adapted from
J.R. Reynolds, Georgia Tech

Why organic semiconductors?

- Processability
  - Vacuum and solution (i.e., printing) deposition
  - Chemistry can be tuned to use different organic solvents and/or water
- Large-area coverage
  - Large-scale printing
- Light weight
- Mechanically flexible, stretchable, & soft

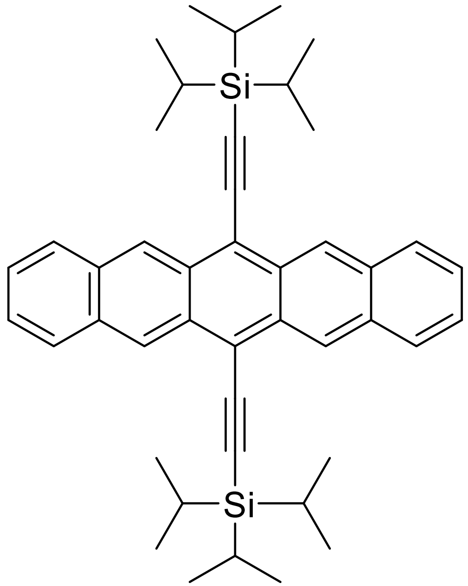
Risø DTU / Grafisk Maskinfabrik

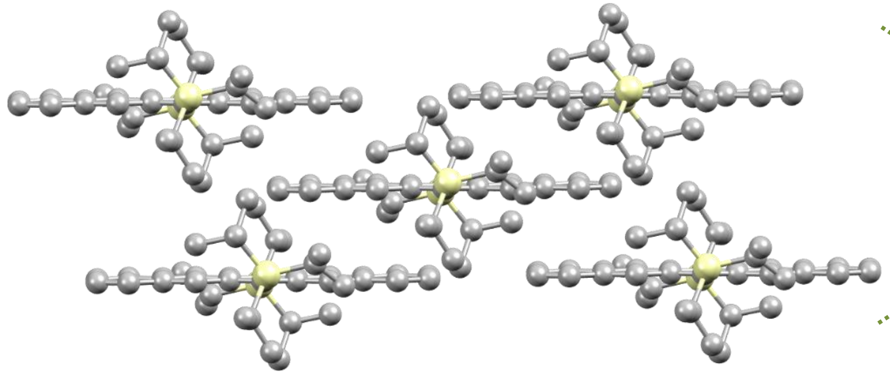
Convergence of materials science, data science, and robotics

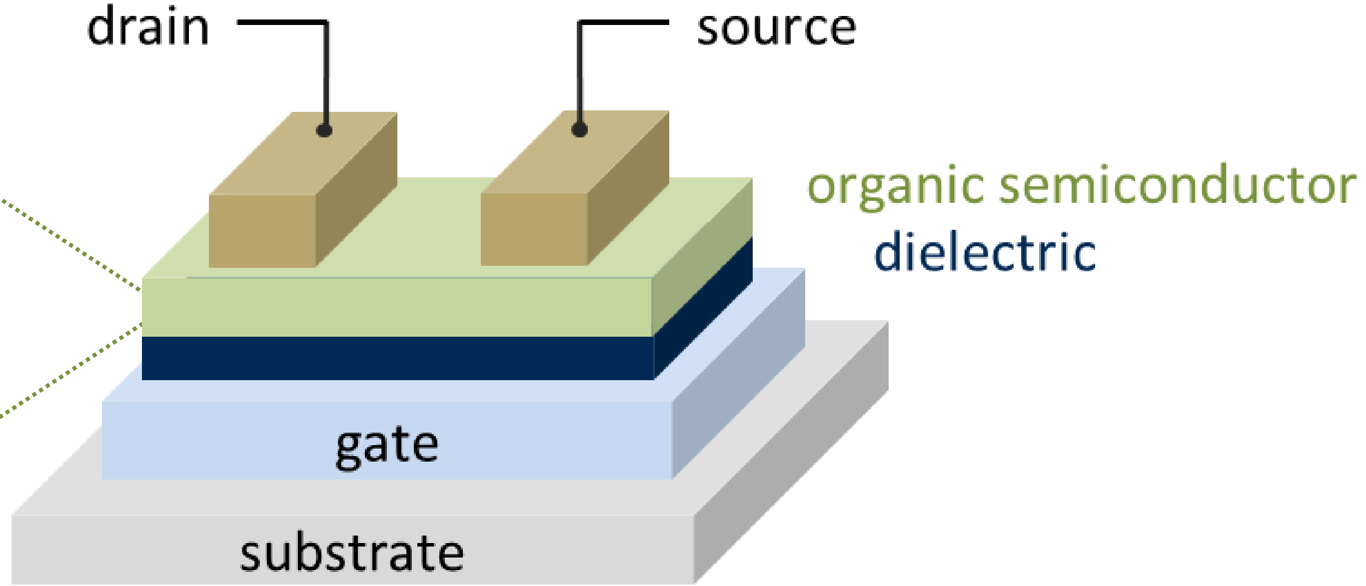


Launched in 2011 to accelerate the discovery, design, development, and deployment of new materials, at a fraction of the cost, by harnessing the power of data and computational tools in concert with experiment.

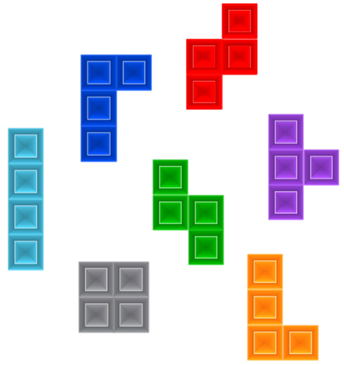
Let’s use the transistor as our application model







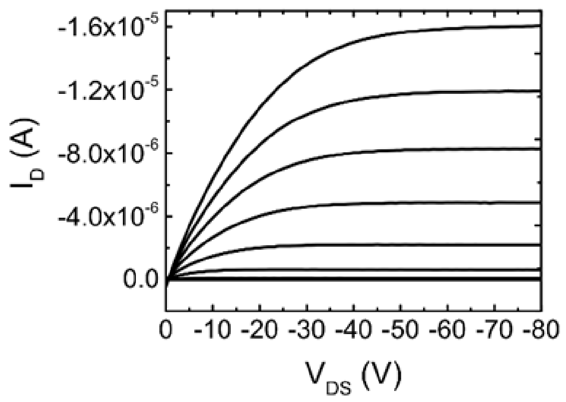
in silico design



A vast chemical space of organic chromophores

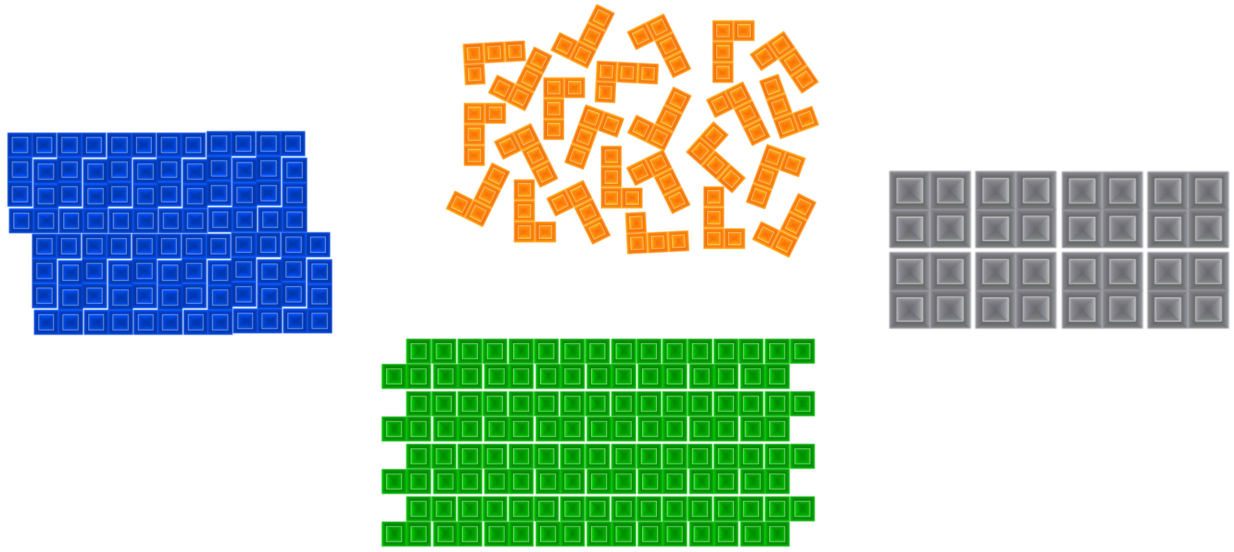
BUILDING BLOCK

?



A. Zeidell *et al*. Chem. Mater. (2019) 31, 6962.

RESPONSE



STRUCTURE & SYNTHESIS PREDICTION

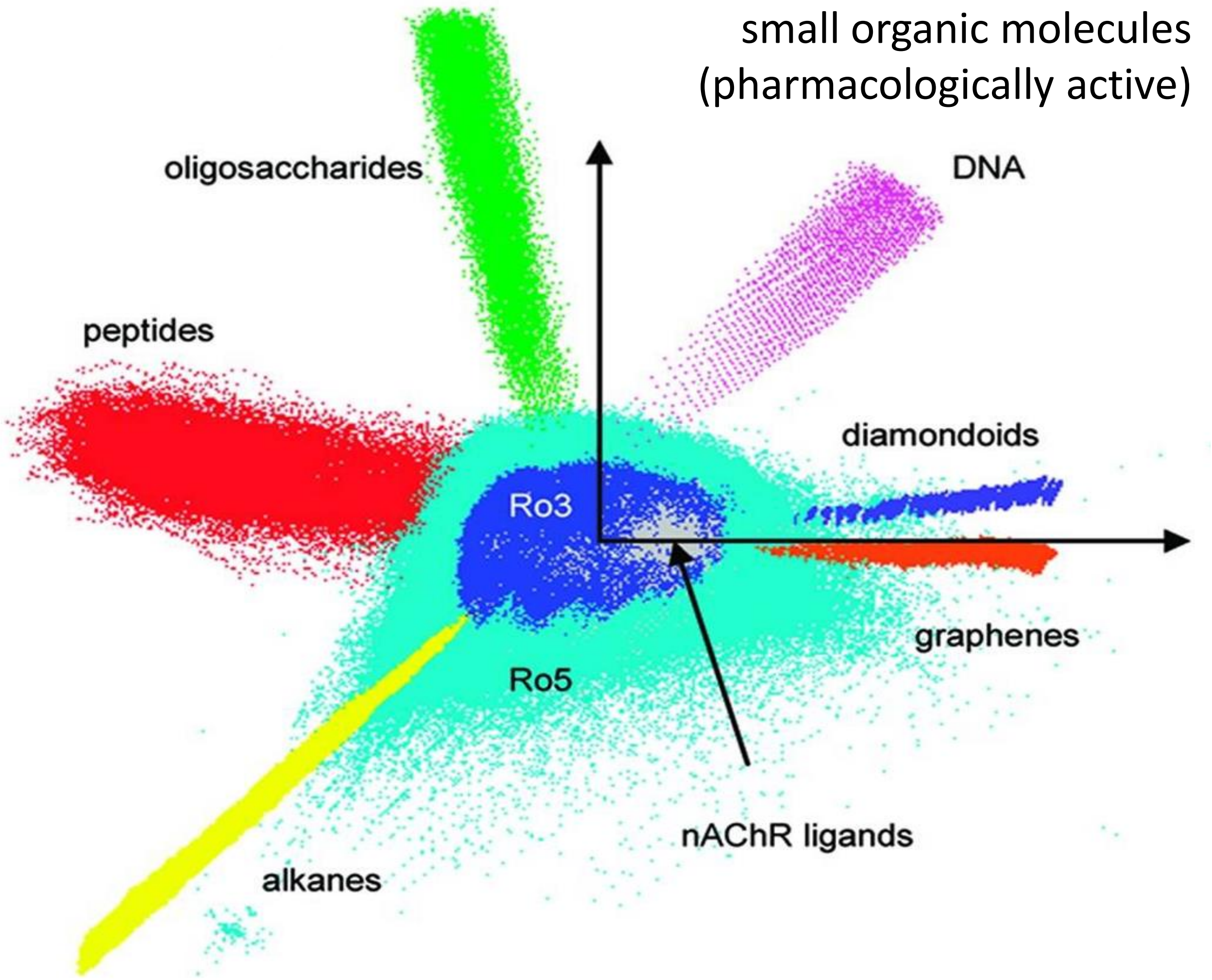
PROPERTY PREDICTION

Adapted from Q. Ai

The chemical space for organic materials is large

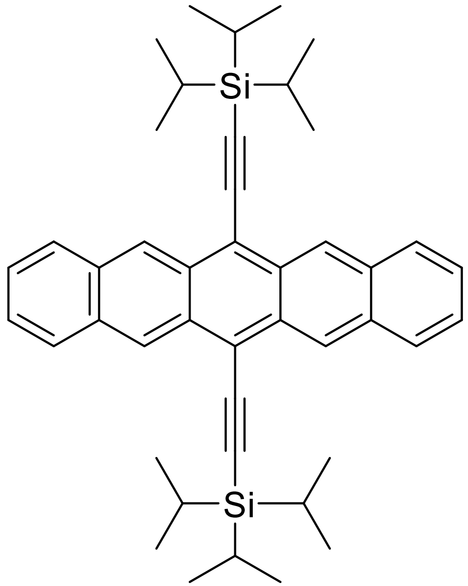
All things considered…chemical space is massive!

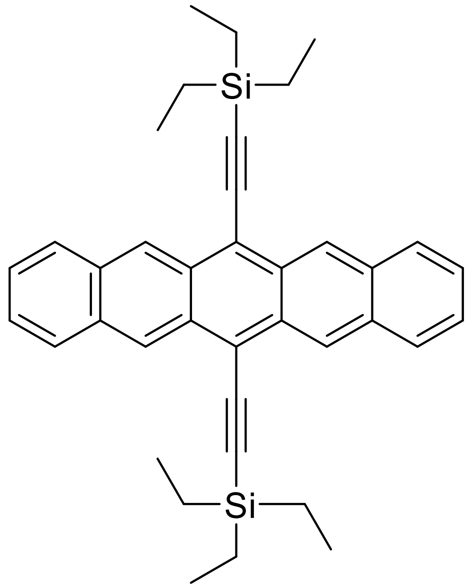
- 10^{18} grains of sand on Earth
- 10^{23} stars in the visible sky
- 10^{60} small organic molecules (pharmacologically active)

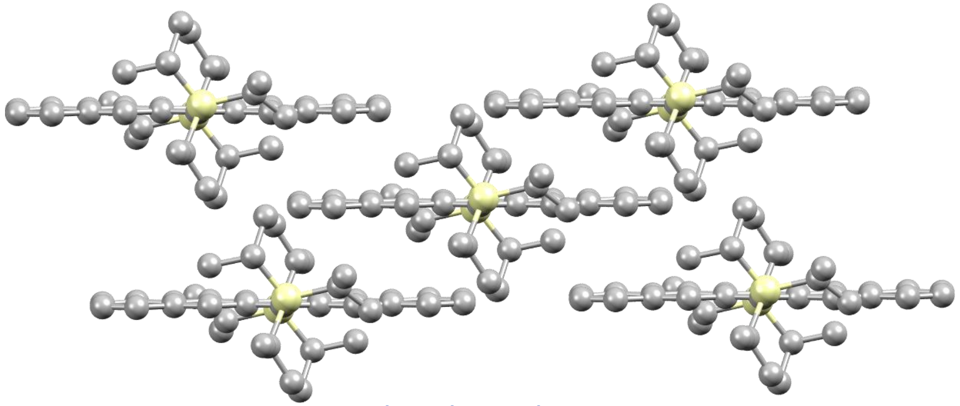


P. Kirkpatrick & C. Ellis, Nature 2004, 432, 823;
C. Lipinski & Andrew Hopkins, Nature 2004, 432, 855;
J.L. Reymond & M. Awale, ACS Chem Neurosci. 2012, 3, 649.

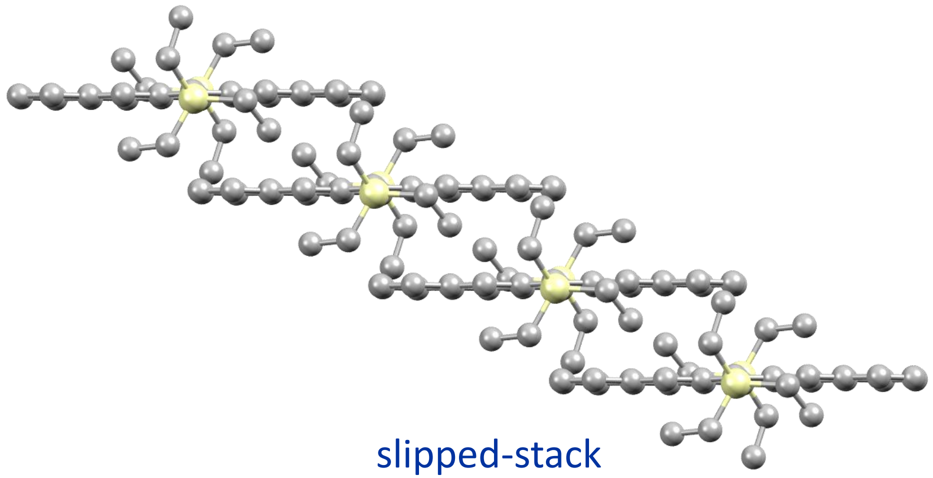
TAS-Pentacene: TIPS v. TES Substituents







brickwork

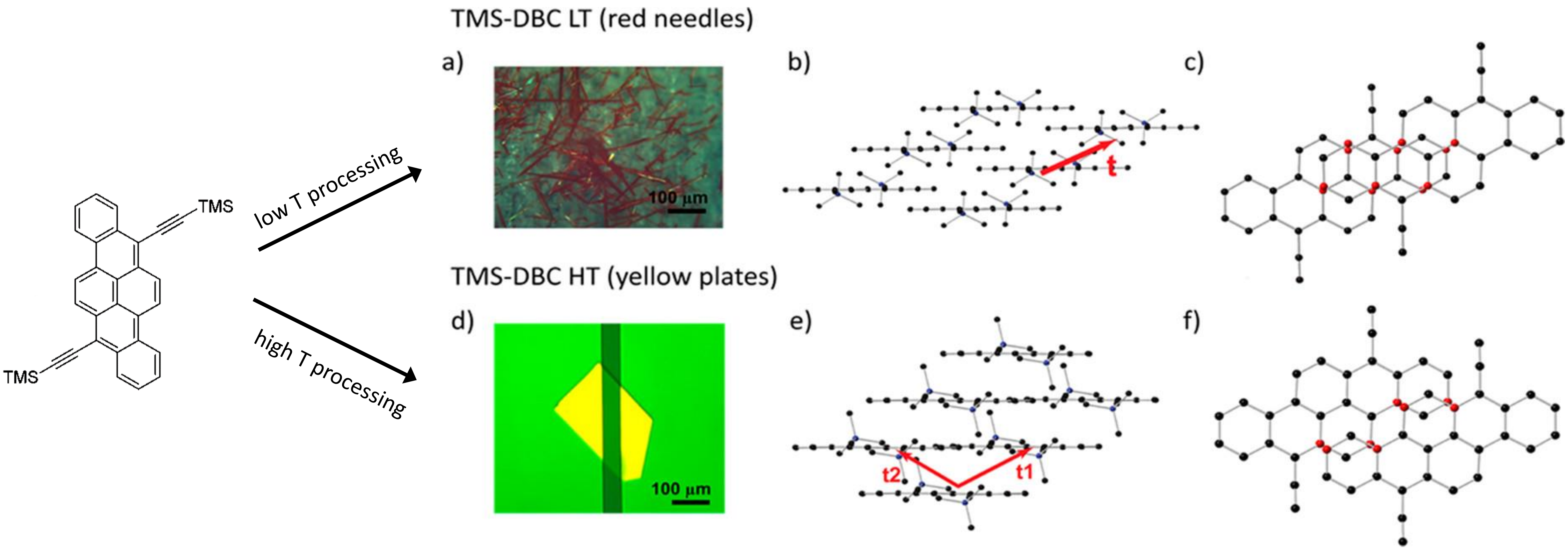


slipped-stack

K.J. Thorley, T.W. Finn, K. Jarolimek, J.E. Anthony, C. Risko, Chem. Mater. 2017, 29, 2502.

Polymorphs and processing

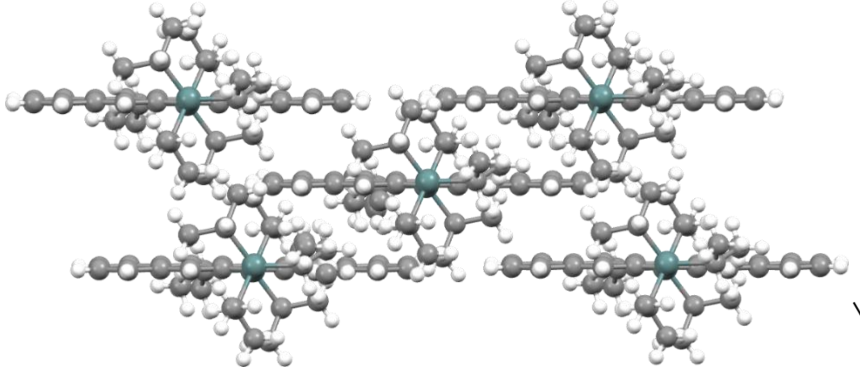
$\mu_h = 0.028\ cm^2V^{-1}\ s^{-1}$



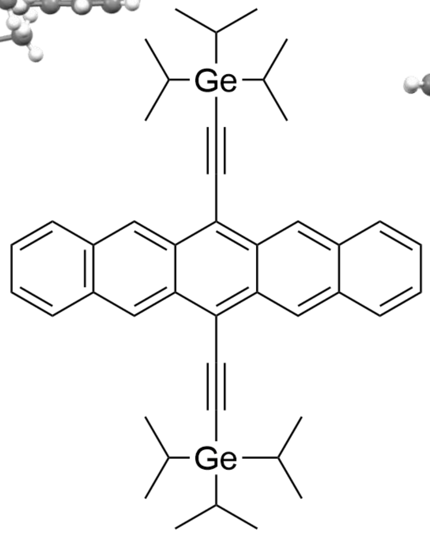
$\mu_h = 2.1\ cm^2V^{-1}\ s^{-1}$

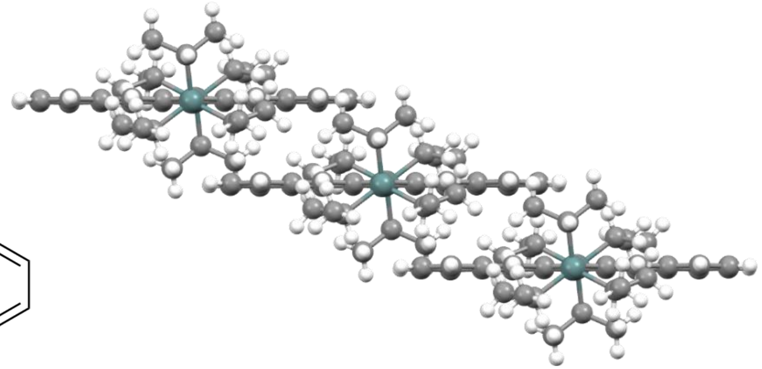
L. Stevens, V. Coropceanu, O.D. Jurchescu, G.E. Collis, et al. Chem. Mater. 2015, 27, 112.

Polymorphs and processing



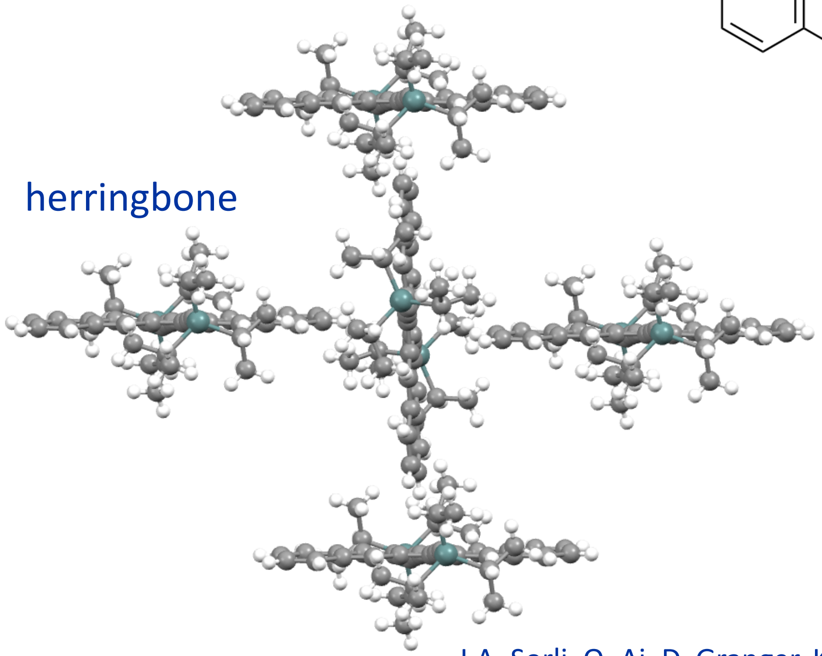
brickwork





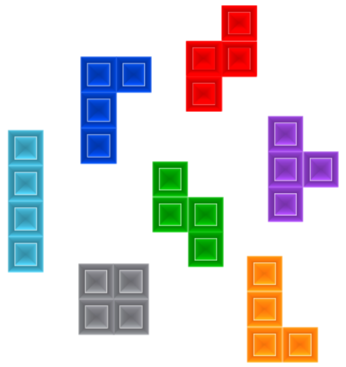
slipped-stack

herringbone



J.A. Sorli, Q. Ai, D. Granger, K. Gu, S. Parkin, K. Jarolimek, N. Telesz, J.E. Anthony, C. Risko & Y.L. Loo, Chem. Mater. 2019, 31, 6615.

in silico design



A vast chemical space of organic chromophores

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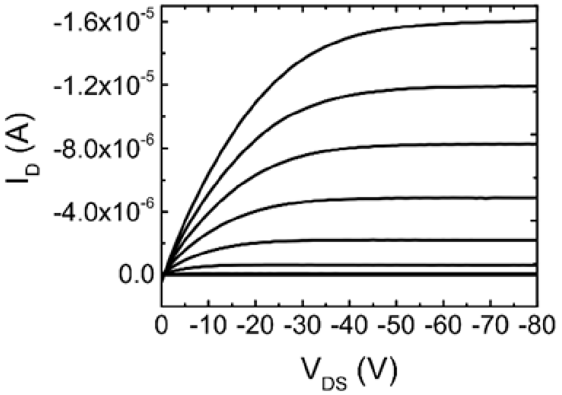
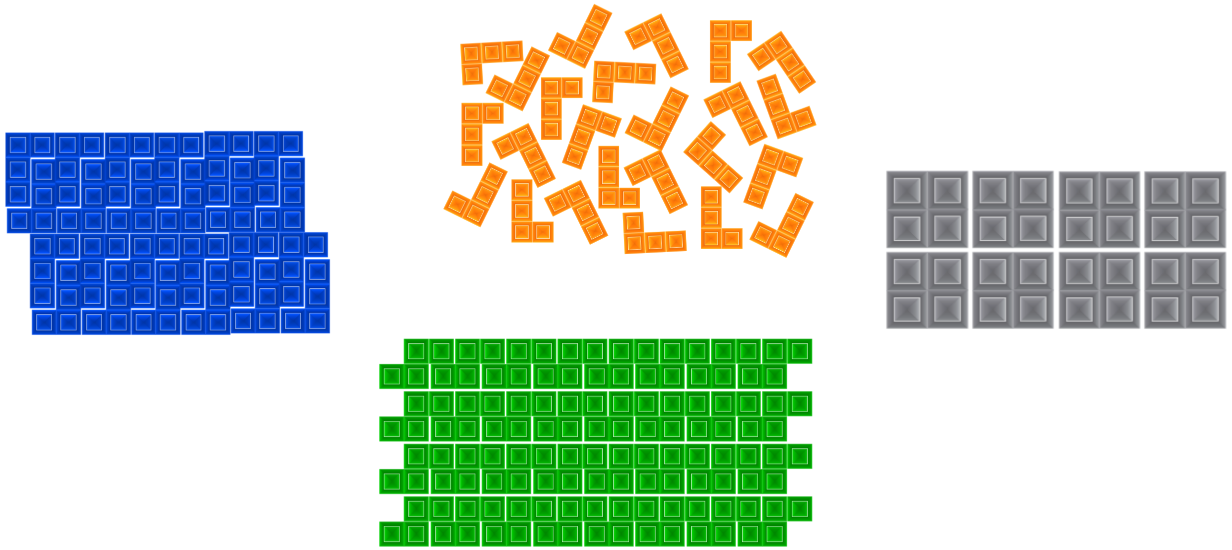


A. Zeidell *et al*. Chem. Mater. (2019) 31, 6962.

RESPONSE



STRUCTURE & SYNTHESIS PREDICTION

PROPERTY PREDICTION

Adapted from Q. Ai

Data structures and data bases

Data is becoming ever more accessible…

Materials Project
AFLOW
NOMAD
Khazana
JARVIS-DFT
Open Quantum Materials Database
Materials Data Facility

do we have enough data?
do we have the "right" data?
can we automate synthesis & characterization?
how do we develop & deploy (semi)autonomous discovery?

…and for organic semiconductors…

Organic Materials Database
electronic and magnetic properties of organic and organometallic materials

Organic Crystal Structure and Electronic Properties Database
electronic bandgaps, band dispersions, and molecular orbital energy gaps

Organic Crystals in Electronic and Light Oriented Technologies (OCELOT)

Open Access infrastructure

oscar.as.uky.edu

56k crystals
47k molecules
38k π-conjugated chromophores

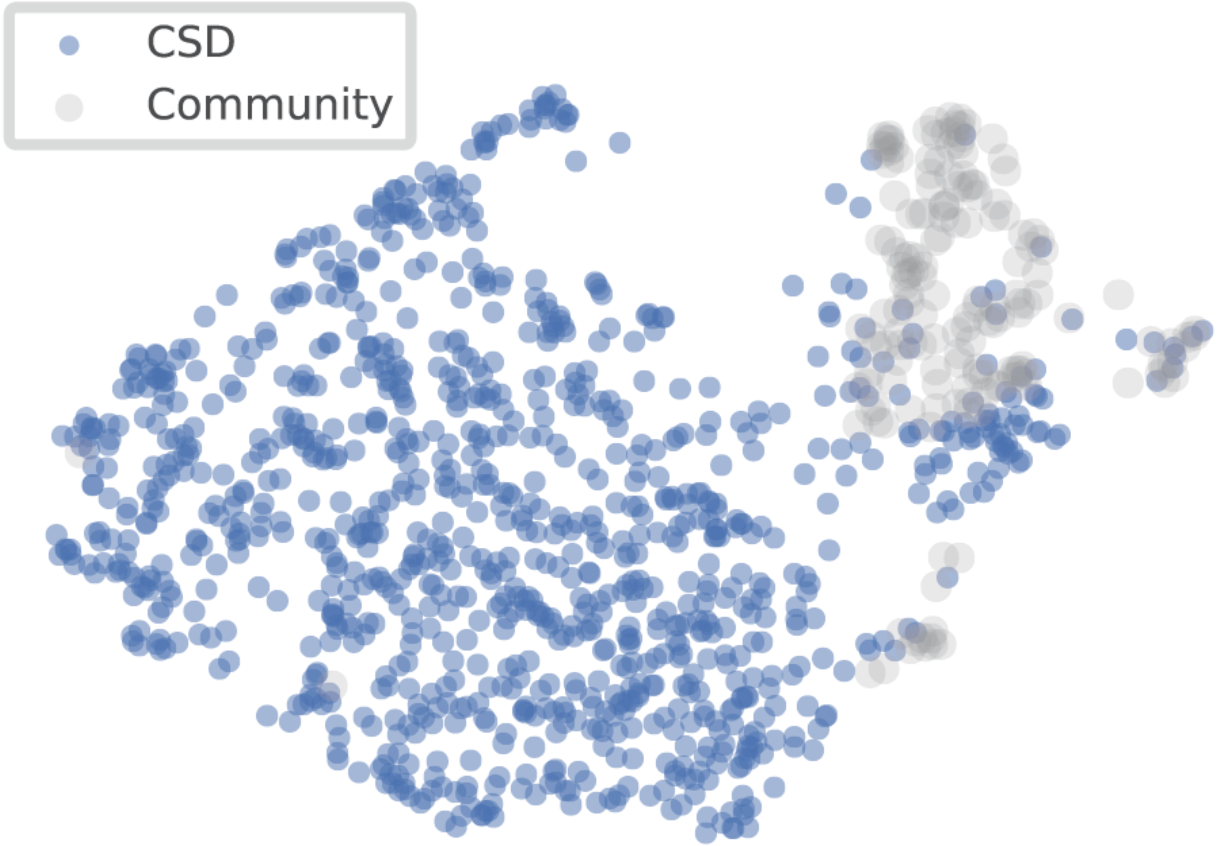
OCELOT

- A Python tool kit for data analysis
- High-throughput computational workflows
- User-friendly web user interface
- Access to machine learning predictions

Q. Ai, V. Bhat, S.M. Ryno, L.Y. Huang, A. Smith, P. Sornberger, R. Duke, S. Goodlett, C. Risko with J.E. Anthony & M.M. Haley;
Q. Ai, V. Bhat, S.M. Ryno, K. Jarolimek, P. Sornberger, A. Smith, M.M. Haley, J.E. Anthony & C. Risko, J. Chem. Phys. 2021, 154, 174705.

Data set includes “dark” structures

- OCELOT contains structures not reported elsewhere – ‘dark’ or missing structures from the literature



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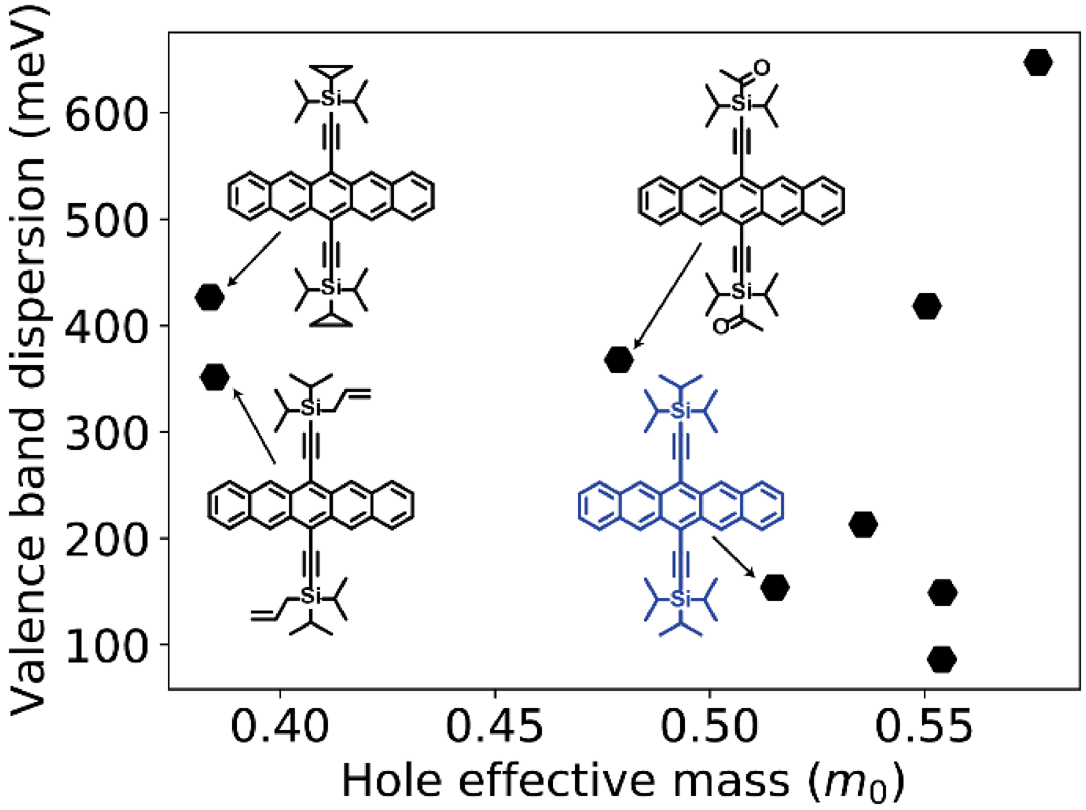
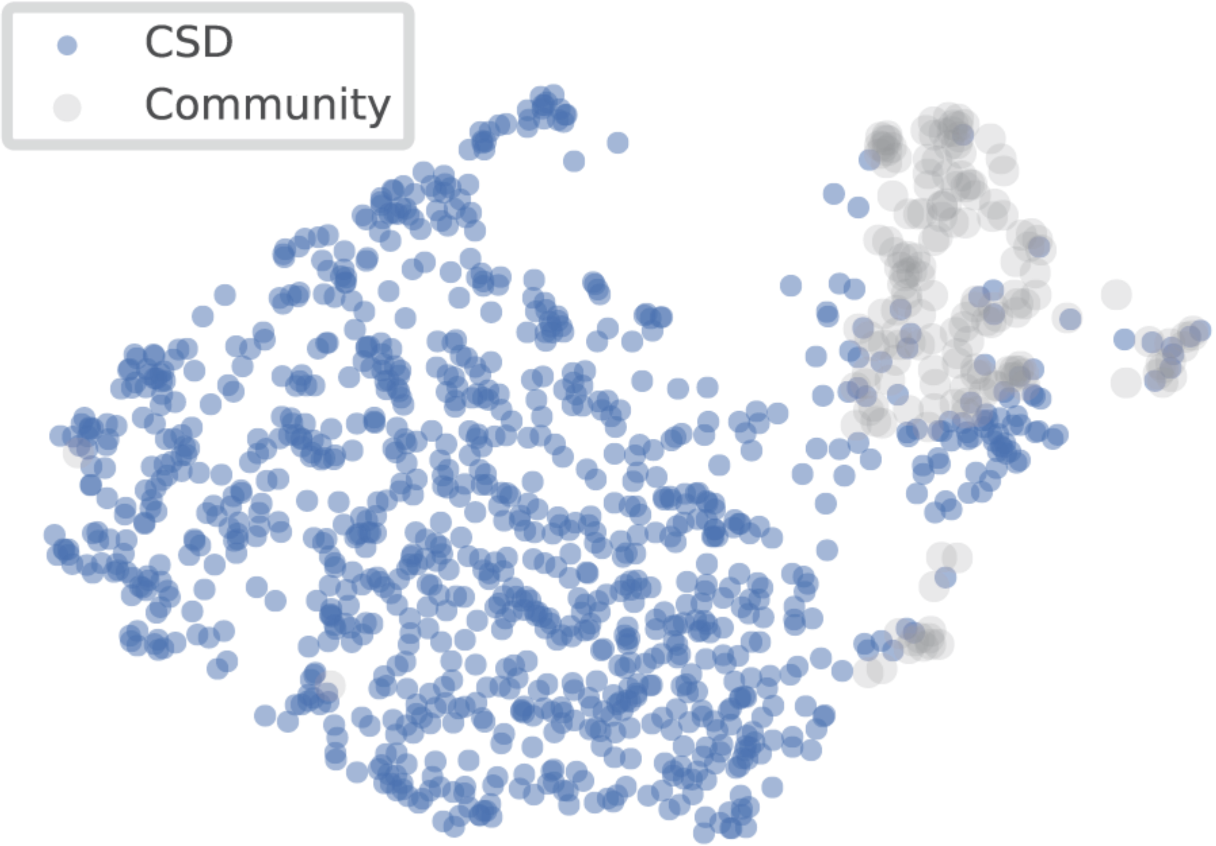
Data set includes “dark” structures

- Inclusion of dark structures aids in further exploration of chemical space of OSC





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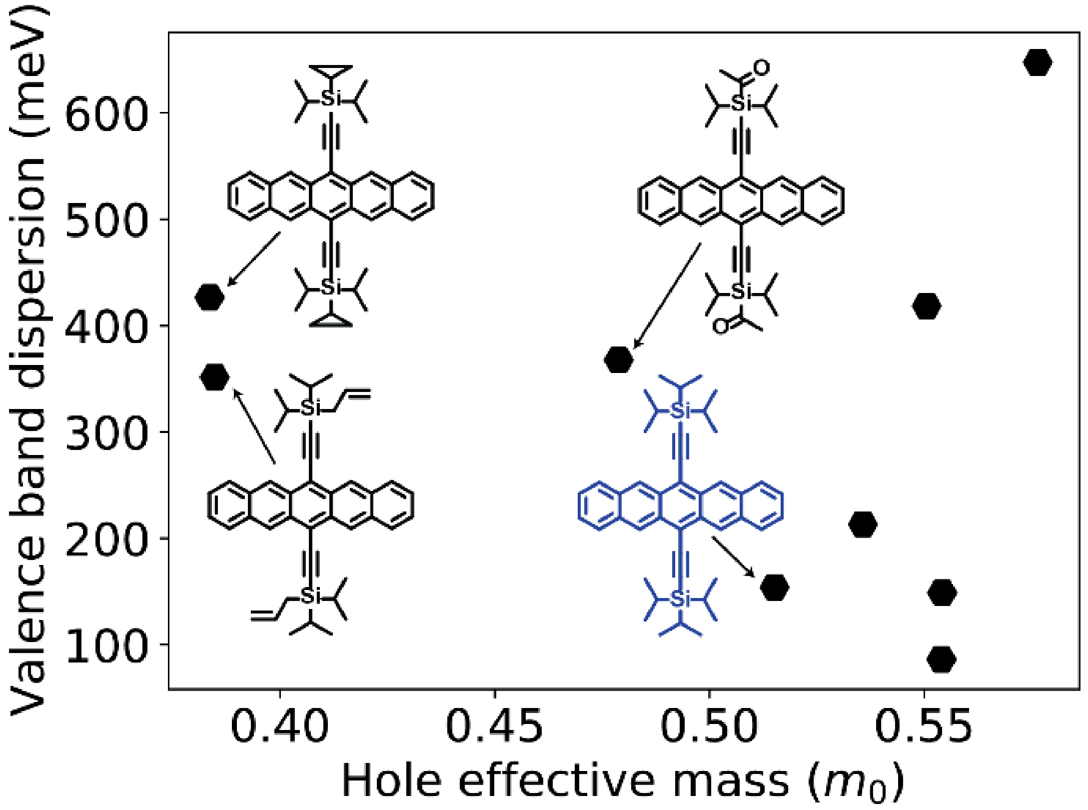

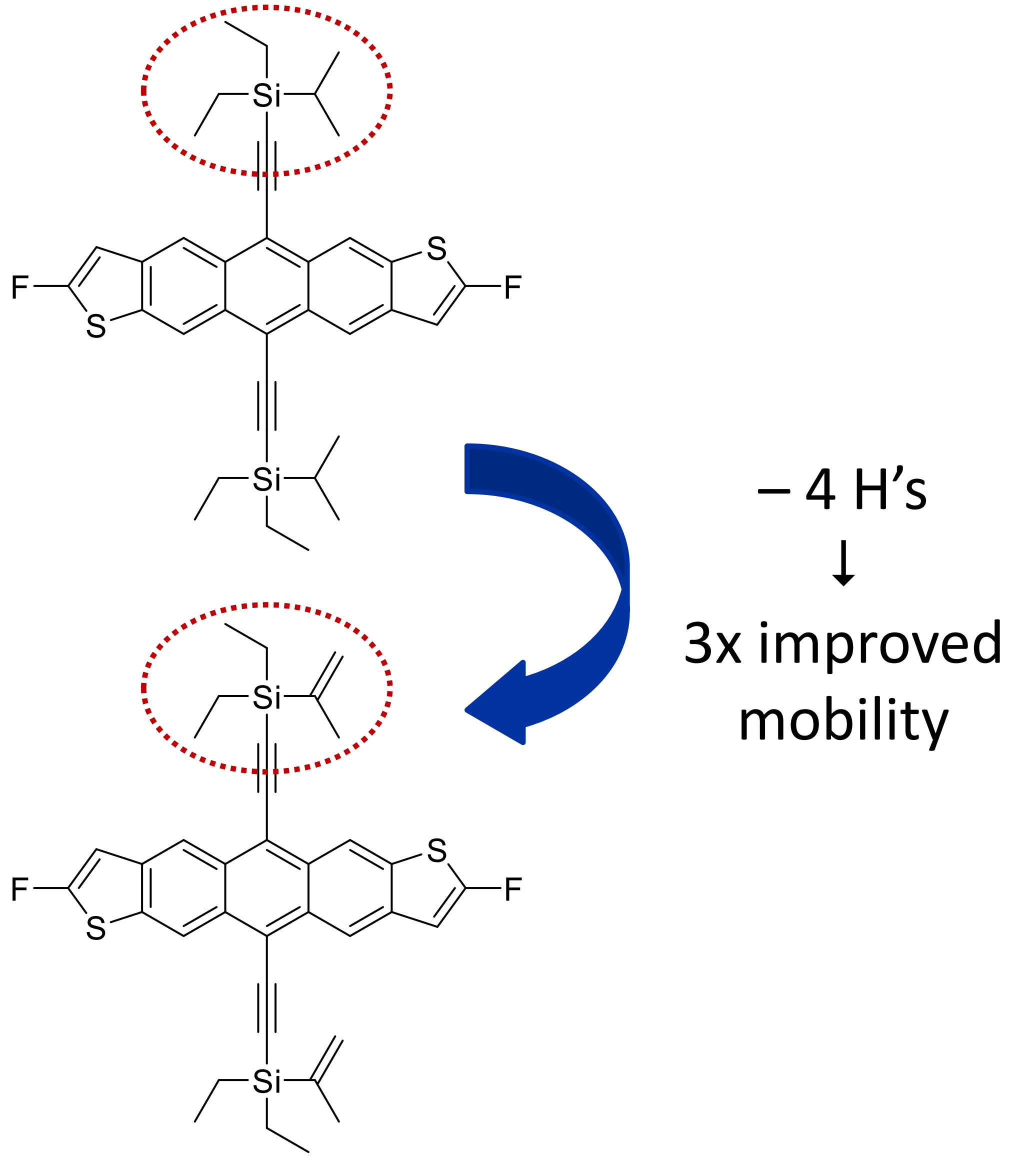

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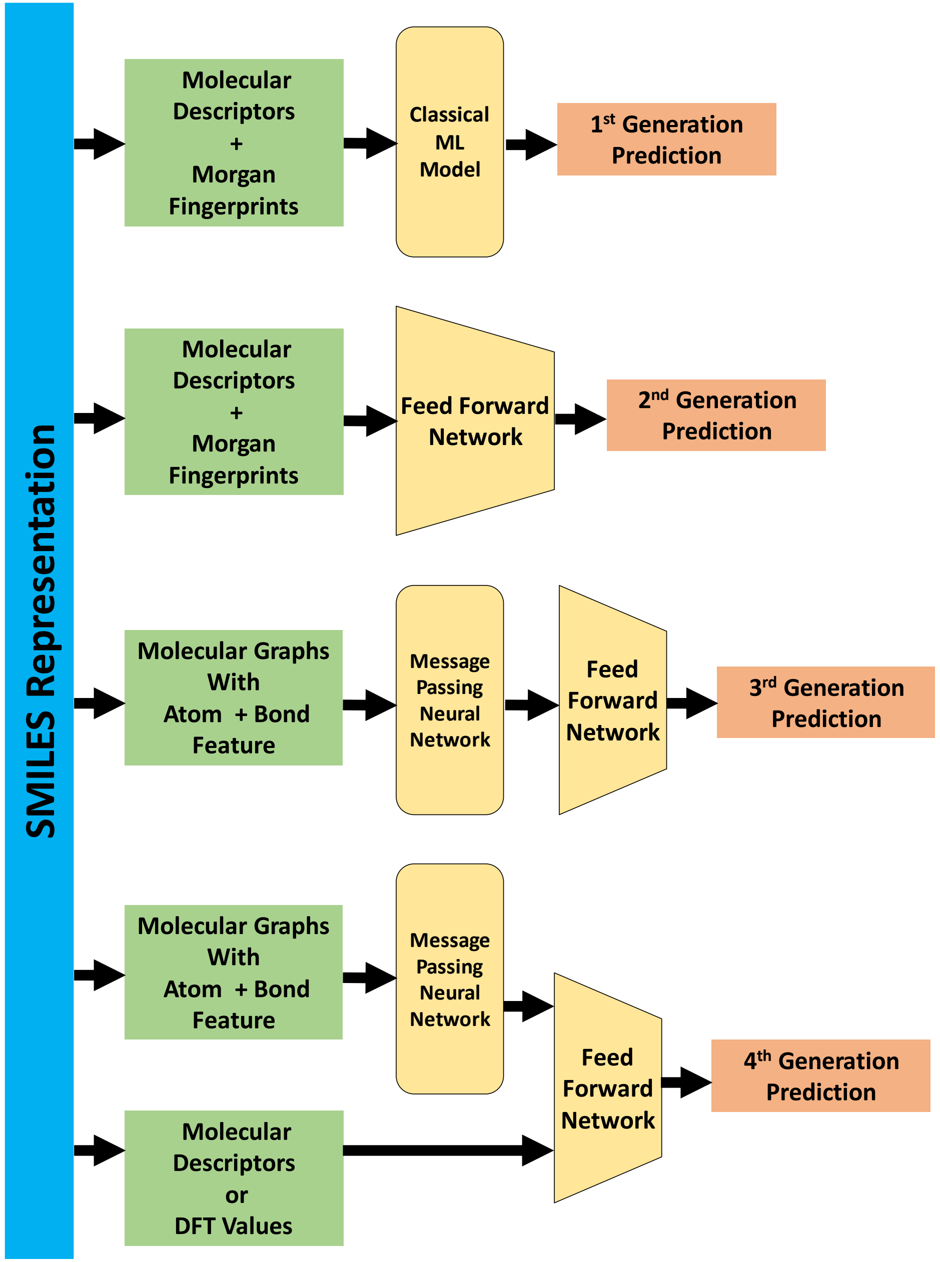
Q. Ai, V. Bhat, S.M. Ryno, K. Jarolimek, P. Sornberger, A. Smith, M.M. Haley, J.E. Anthony & C. Risko, J. Chem. Phys. 2021, 154, 174705.

Let's predict molecular & materials properties



- Challenges that need to be overcome:
  - Computing DFT-based electronic properties is time consuming
  - Recently published models are trained on datasets with ~25 atoms or rather niche chemical space

- Properties modeled:

  Vertical (VIE) and adiabatic (AIE) ionization energies
  Vertical (VEA) and adiabatic (AEA) electron affinities
  Cation (CR) and anion (AR) relaxation energies
  HOMO energies (HOMO), LUMO energies (LUMO)
  HOMO-LUMO energy gaps (H-L)
  Electron (ER) and hole (HR) reorganization energies
  Lowest-lying singlet (S0S1) and triplet (S0T1) excitation energies

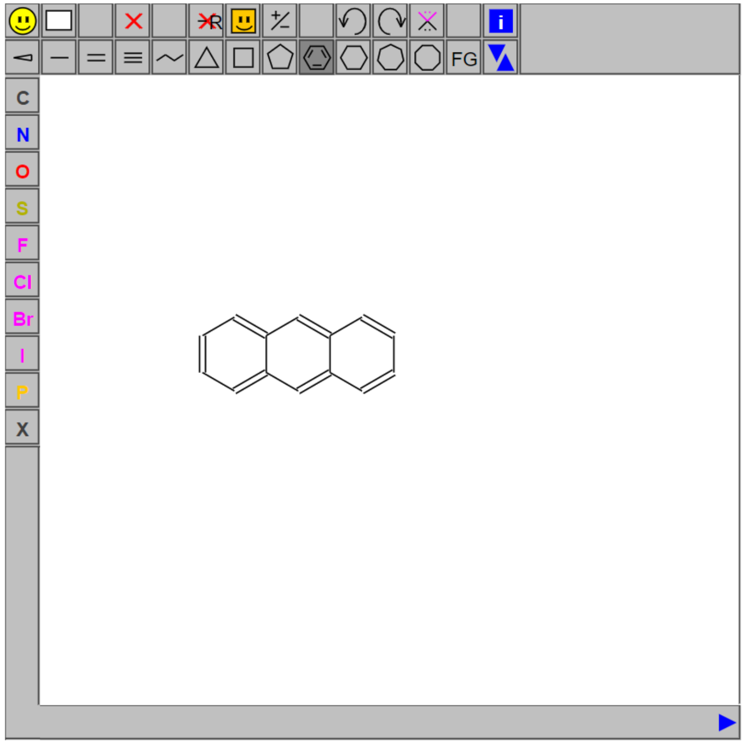
OCELOT ML

oscar.as.uky.edu/ocelotml_2d

V. Bhat, P. Sornberger, B. Pokuri, R. Duke, B. Ganpathysubramanium & C. Risko, Chem. Sci. (2023), 14, 203;
V. Bhat, B. Ganapathysubramanian & C. Risko, (2023) ChemRxiv, DOI: 10.26434/chemrxiv-2023-rvzmv.

Let’s predict molecular & materials properties

- OCELOT ML provides the infrastructure to make the models publicly accessible
- Currently, molecular predictions with SMILES input is supported
- Best models from our training are available



OCELOT ML

oscar.as.uky.edu/ocelotml

Select propety to predict

Adiabatic Ionization Energy (R2 = 0.87; MAE = 0.16)

Predict

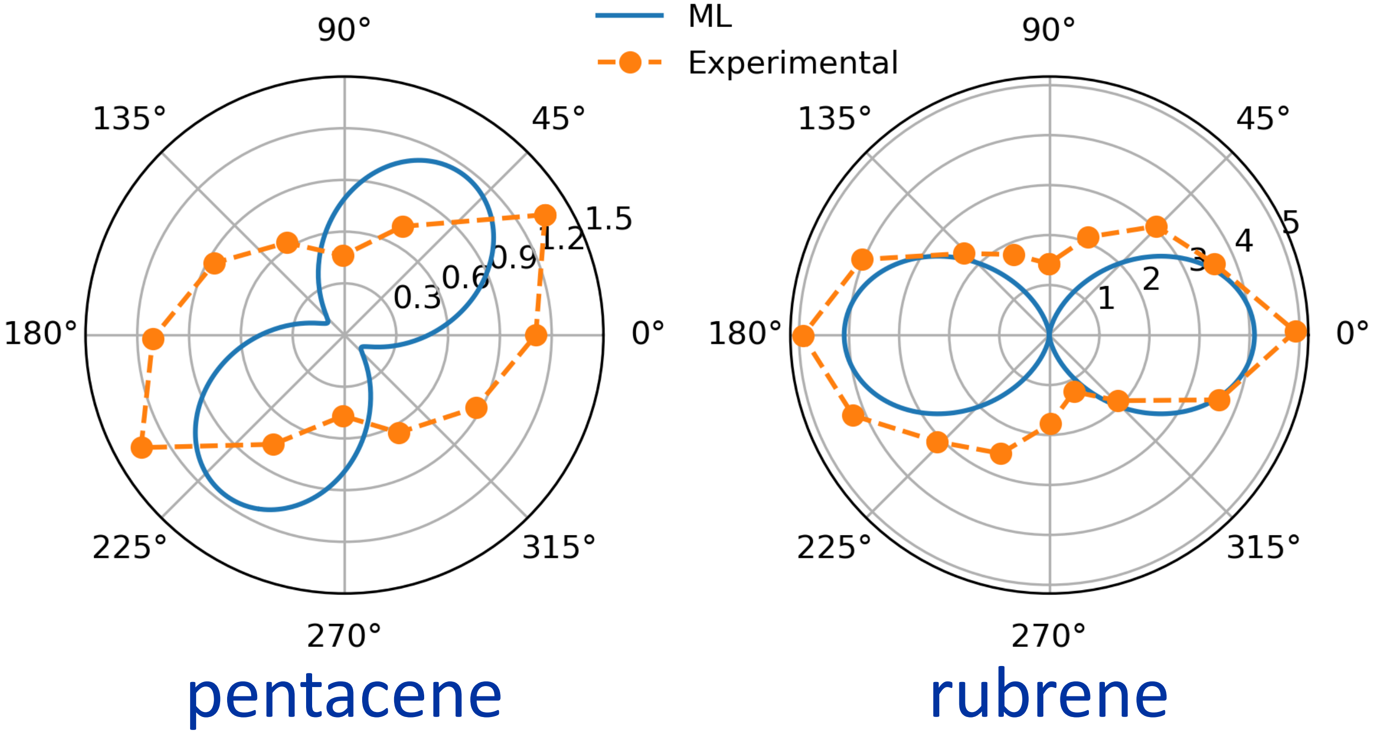
Predicted value is : 7.16 ± 0.151 eV

V. Bhat, P. Sornberger, B. Pokuri, R. Duke, B. Ganpathysubramanium & C. Risko, Chem. Sci. (2023), 14, 203.

Let's predict molecular & materials properties

via semi-empirical Marcus theory, prediction of charge-carrier mobility anisotropy

- ML intramolecular reorganization energy
- ML intermolecular electronic couplings



OCELOT ML

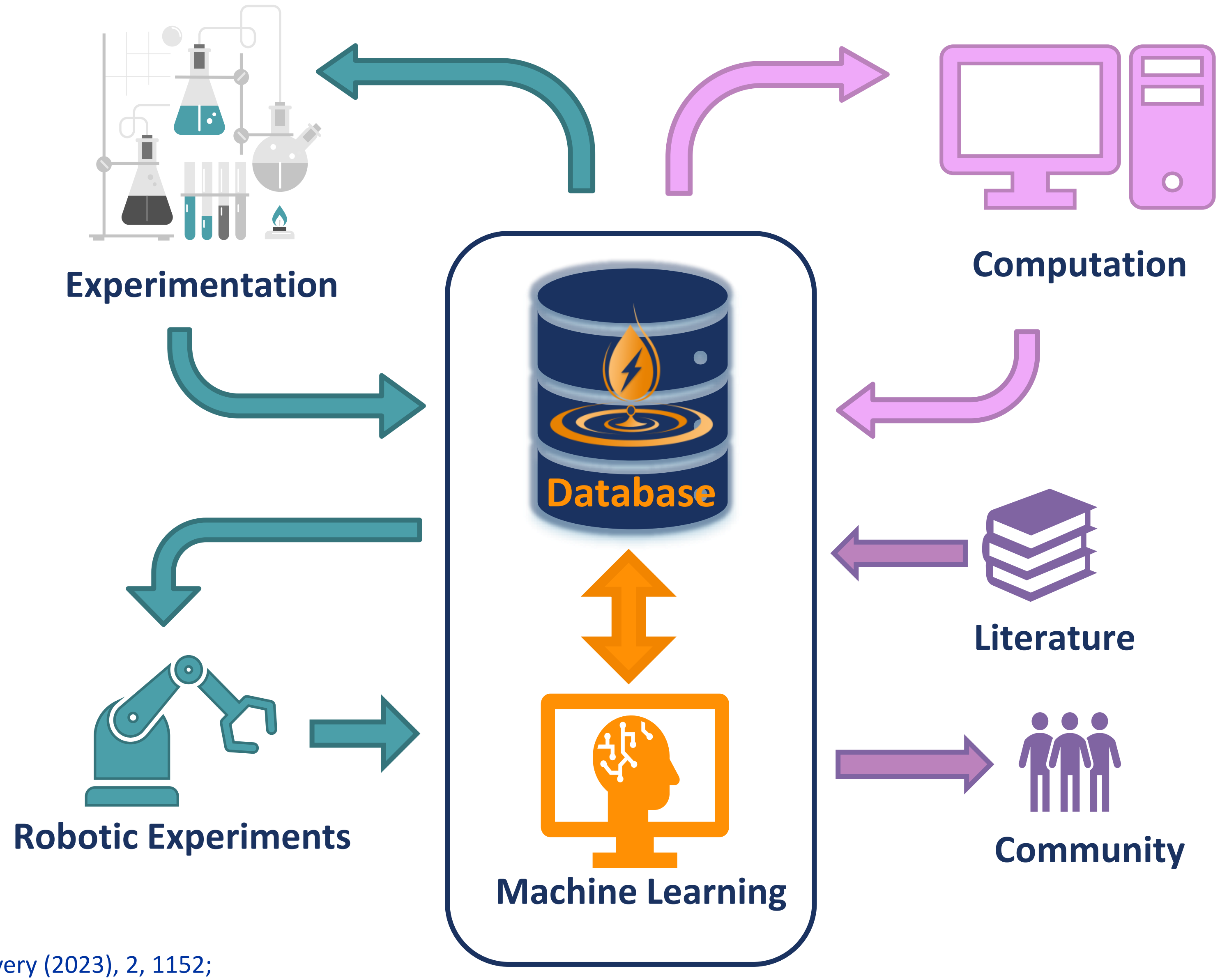
oscar.as.uky.edu/ocelotml

V. Bhat, B. Ganapathysubramanian & C. Risko, (2023) ChemRxiv, DOI: 10.26434/chemrxiv-2023-rvzmv;
V. Bhat, Q. Ai, & C. Risko, Provisional Patent Application 63/4888713

Now on to materials for batteries

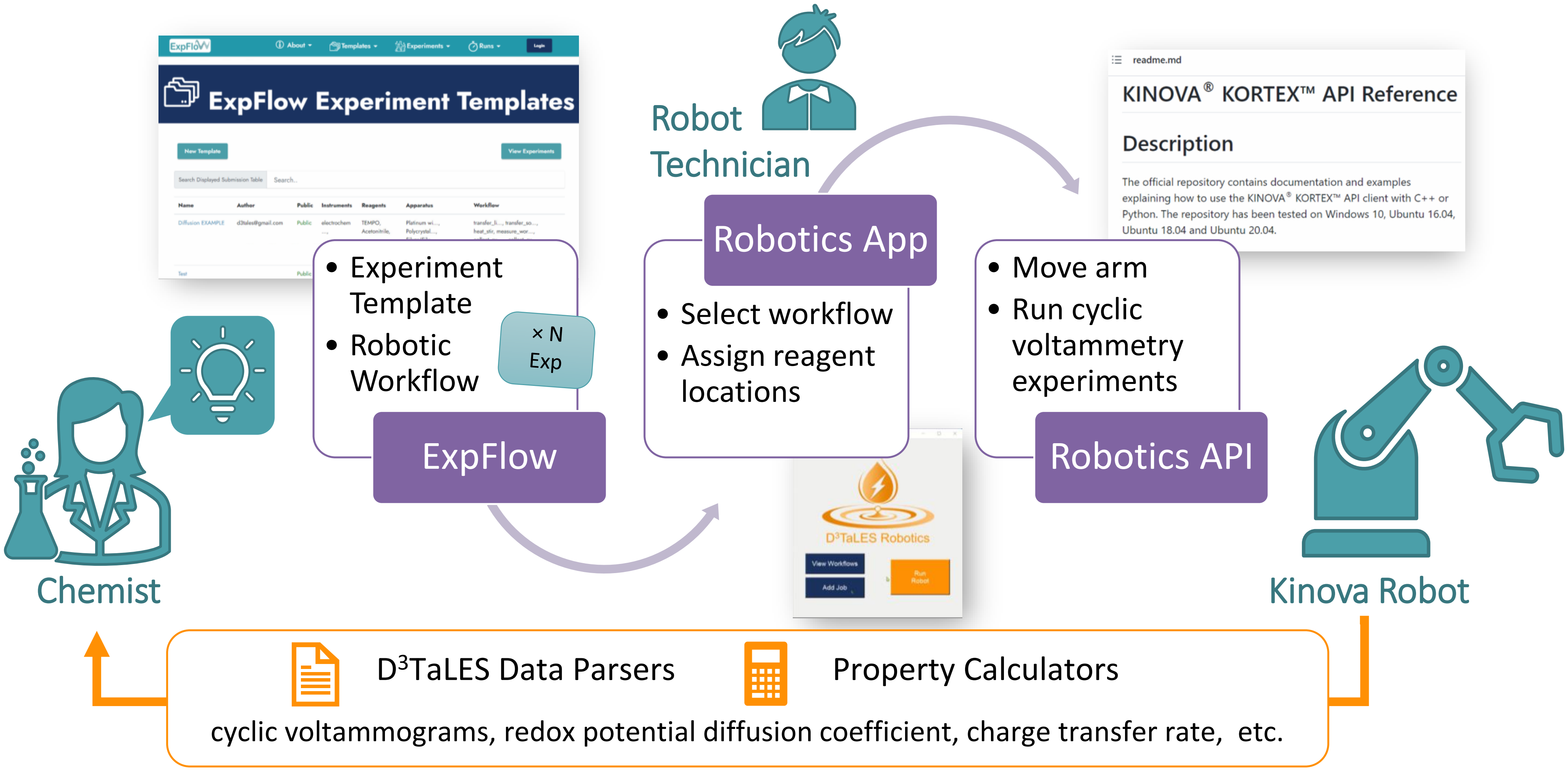
Data-enabled **D**iscovery and **D**esign to **T**r**a**nsform **L**iquid-based **E**nergy **S**torage (D^{3}TaLES)

d3tales.as.uky.edu



R. Duke, V. Bhat, P. Sornberger, S.A. Odom & C. Risko, Digital Discovery (2023), 2, 1152;
R. Duke, S. Mahmoudi, A.P. Kaur, V. Bhat, I. Dingle, N.C. Stumme, S.K. Shaw, D. Eaton, A. Vego & C. Risko, Digital Discovery (2024), 3, 163.

Automated electrochemistry



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Automated electrochemistry

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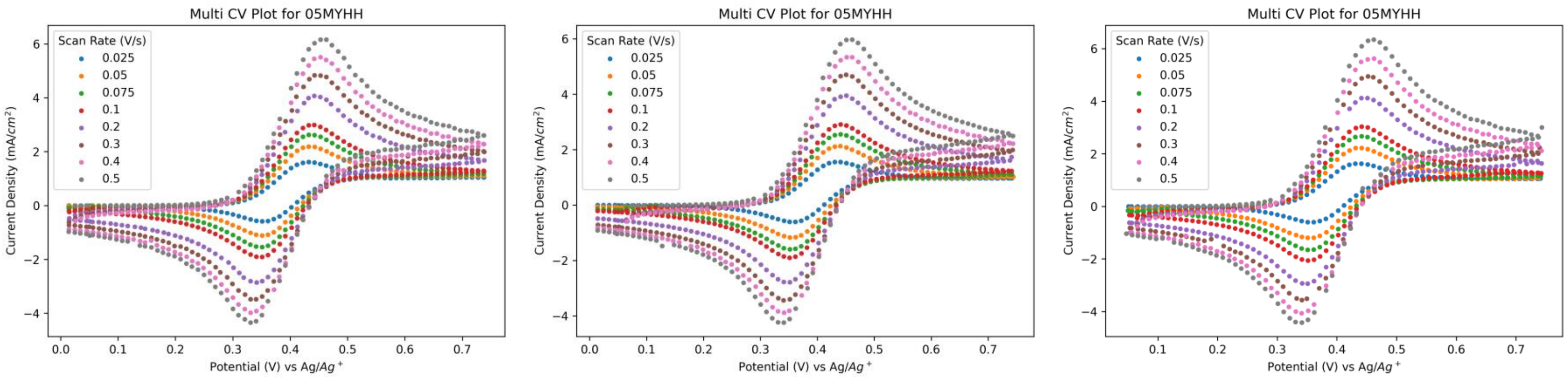
Automated electrochemistry

N-[2-(2-methoxyethoxy)ethyl]-phenothiazine (MEEPT)

Trail 1 | Trial 2 | Trial 3



	Robotic/ExpFlow						Literature Reported vs. Ag/Ag+		Literature Reported vs. Fc/Fc+	
ROM	Trial 1	Trial 2	Trial 3	Avg. (vs. Ag/Ag^{+})	Std. Dev.	vs. Fc/Fc^{+} [α]	Value	Ref.	Value	Ref.
Fc	0.081	0.082	0.082	0.082	0.001	0.000	0.086	Ref.[6]		
MEEPT	0.396	0.396	0.396	0.396	0.000	0.314	0.410*	Ref.[14]	0.310	Ref.[8]
DMPZ	-0.156	-0.156	-0.156	-0.156	0.000	-0.238	-0.150	Ref.[9]		
4-MeO TEMPO	0.371	0.376	0.375	0.374	0.003	0.292	0.68[++]	Ref.[5]		
DBB	0.773	0.773	0.773	0.773	0.000	0.691	0.710	Ref.[10]		
DBBB	0.773	0.768	0.773	0.771	0.003	0.690			0.60[‡]	Ref.[13]
TH	0.910	0.910	0.910	0.910	0.000	0.828	0.900	Ref.[12]	0.840	Ref.[7]
ECZ**	0.678	0.678	0.672	0.676	0.003	0.594				

R. Duke, V. Bhat, P. Sornberger, S.A. Odom & C. Risko, Digital Discovery (2023), 2, 1152;
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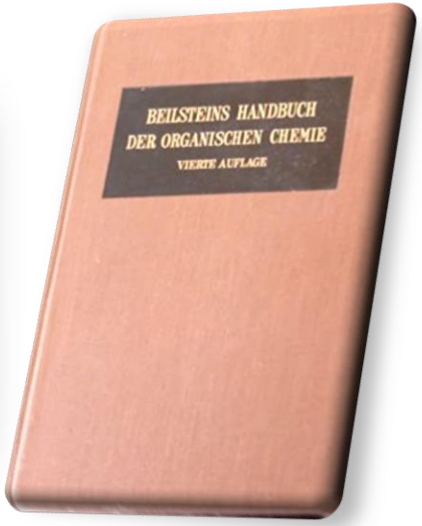
"Big data" in chemistry

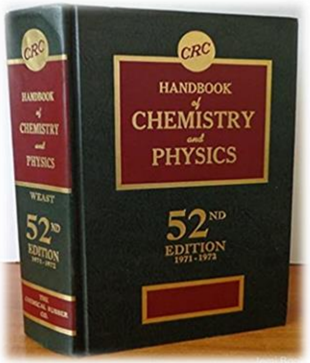
19th century

- Beilstein Handbook of Organic Chemistry[1]
- Gmelin Handbook of Inorganic Chemistry[2]
- Journals and periodicals[3]



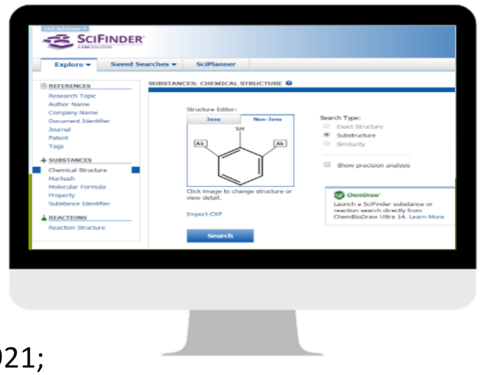
20th century

- Chemical Rubber Company (CRC) Handbook[4]
- The Color Books[5]



21st century

- Web of Science[6]
- SciFinder[6]
- Reaxys[6]



R. Duke, R. McCoy, C. Risko & J.R.S. Bursten. Journal of the American Chemical Society (2024), accepted. DOI: DOI: 10.1021/jacs.3c11399

1) J Chem Inf Comput Sci. 1981, 21, 82; 2) Organometallics 1984, 3, 948; 3) Armour institute of technology , 1919, but not published as a thesis., 1921;
4) Broad, W. J. Rubber Bible Turns 60. Science 1979, 204, 1181; 5) Chem Int. 2017, 39, 2; 6) J. Chem. Educ. 2019, 96, 2167.

THANK YOU!