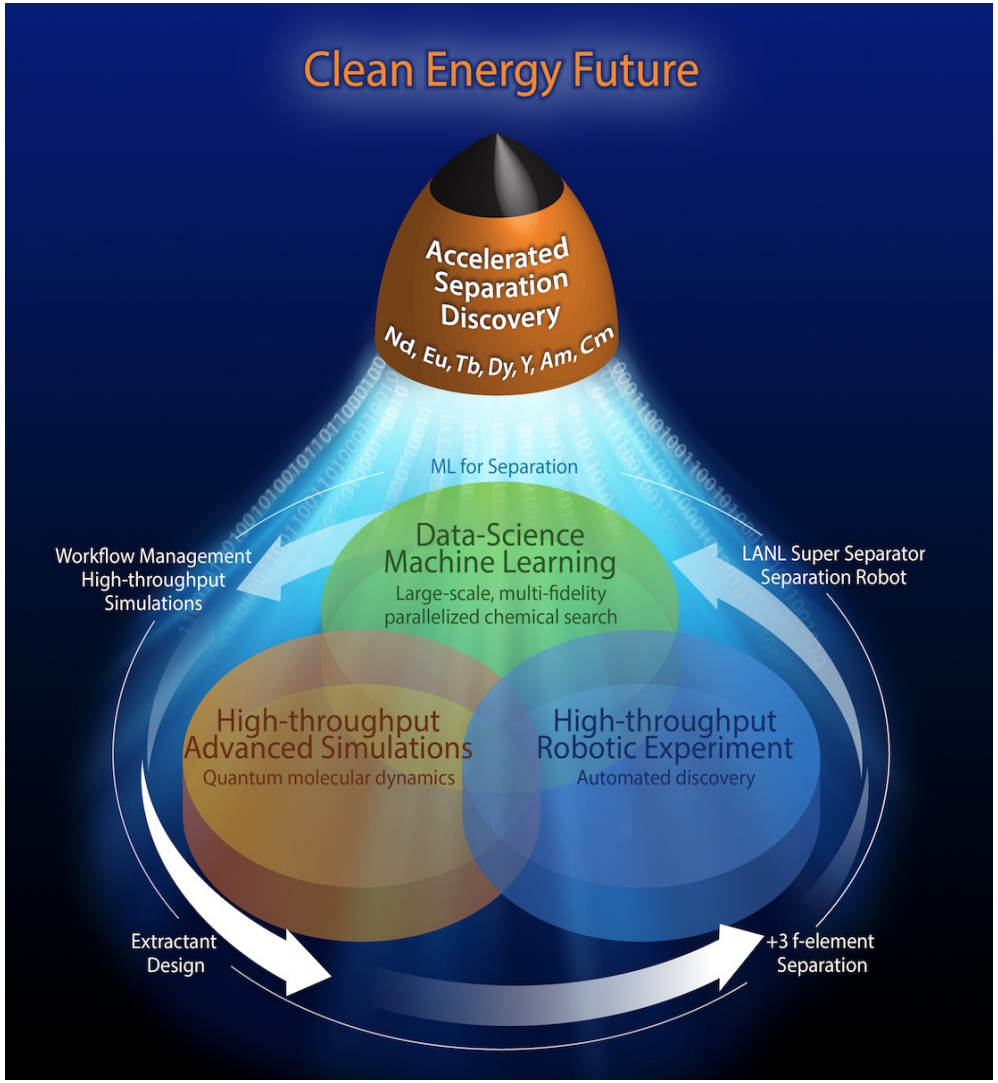
Autonomous Discovery of Separation Science



Ping Yang
Los Alamos National Laboratory

Workshop III: Complex Scientific Workflows at Extreme Computational Scales

Part of the Long Program
New Mathematics for Exascale

IPAM, UCLA

May 1-5, 2023

National Nuclear Security Administration
Managed by Triad National Security, LLC for the U.S. Department of Energy's NNSA

LA-UR# 22-21082

Chemical Separation & Clean Energy

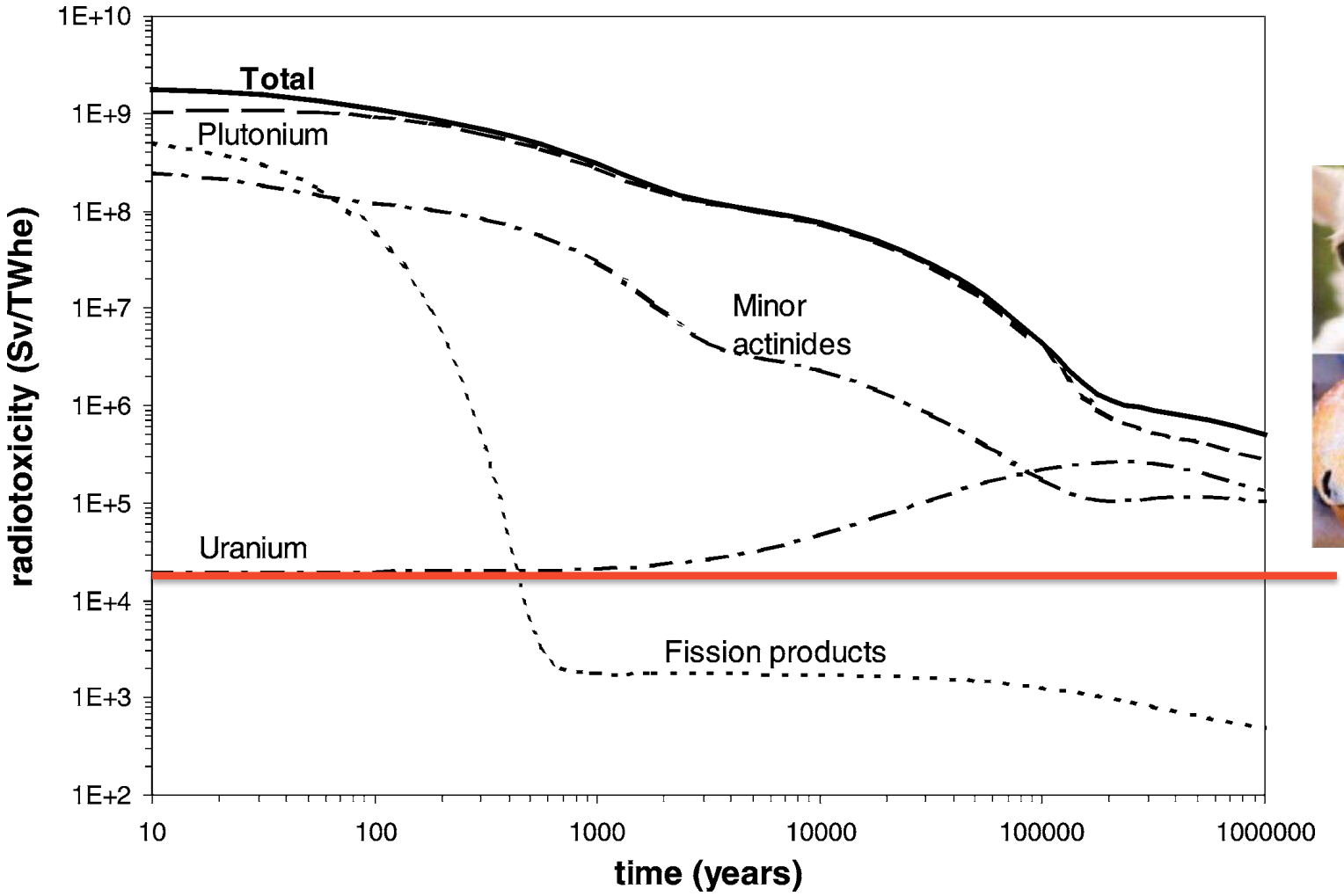
Chemical Separations:

- Critical to almost every aspect of our daily lives from energy, the medications, to clean water
- Costs ~10 – 15% of total energy used in US

Clean Energy and Nuclear Energy:

- Rare-Earth Elements (Nd, Ho, Dy, Eu, etc) needed for clean energy technology, such as wind turbines, EV motors, etc.
- CO_2 level → 420ppm, NE is a low-carbon footprint solution
- 20% of nation's electricity (55% of clean energy in US)
- 80,000+ metric tons of used nuclear fuel in US
- 2,000 metric tons increase each year
- ~$$B annually to deal with the waste
- More nuclear reactors under construction worldwide

Radiotoxicity

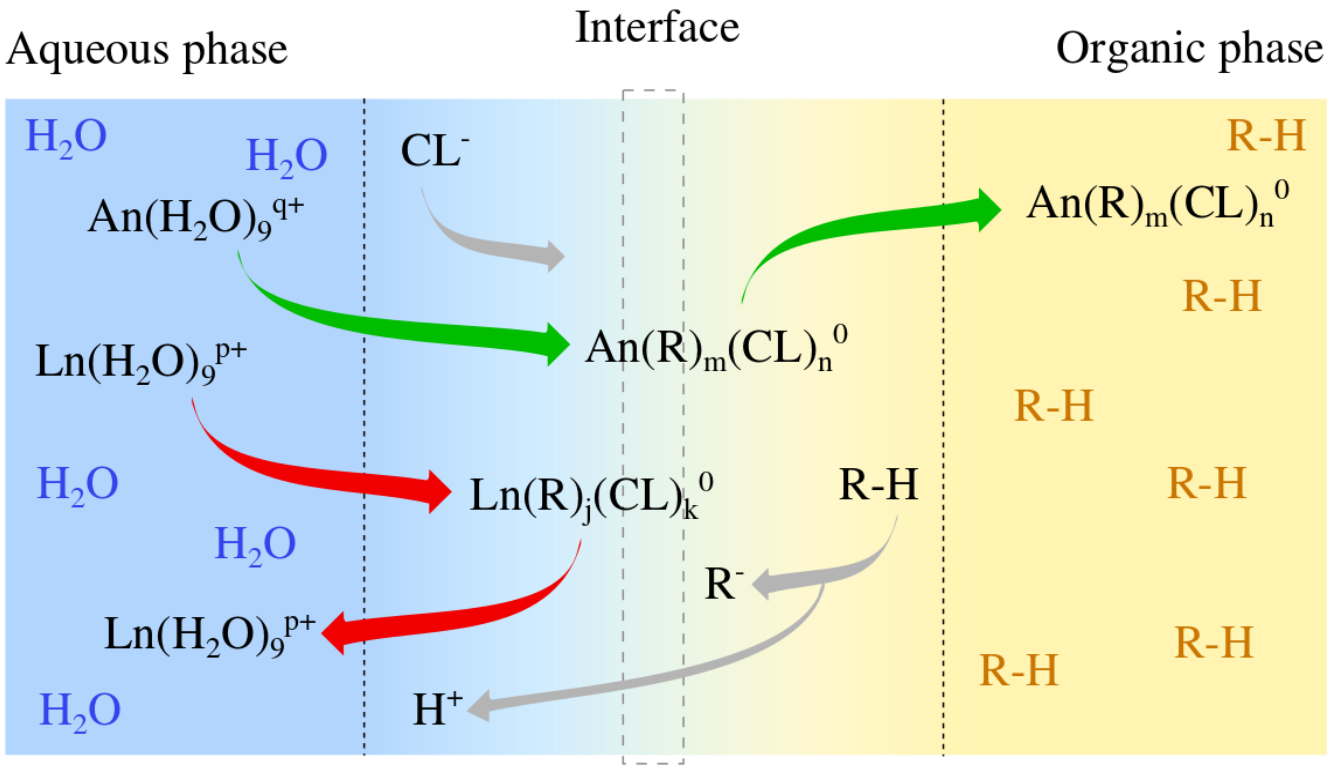


An^{3+}

Ln^{3+}

Madic, C. *et al,* C.R. Physique, 3, 797-811 (2002)

An/Ln and Ln/Ln Solvent Extraction Process



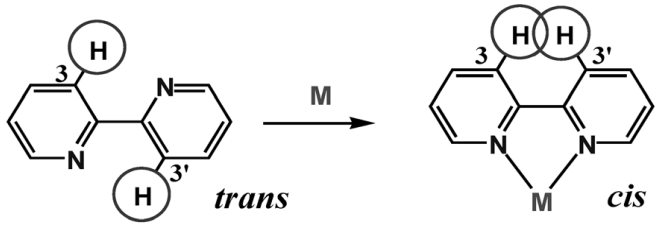
Challenges: chemical space is too vast to be manually explored by experiment or theory.

- Aqueous matrix
- Extractant solubility
- Binding kinetics
- Complexation stability
- Organic matrix
- Phase transfer catalysts
- Matrix effect (cooperative *vs.* blocked binding)
- Holdback agent
- Binding capacity
- Valence adjustment agent and rate
- Resin identity
- Bead size
- Solid-state support properties

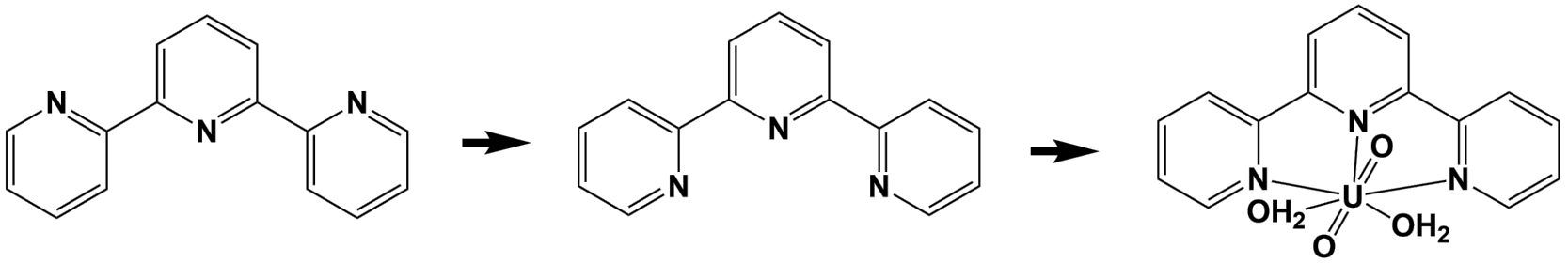
The Conventional Way of Discovering a New Extractant

Starting with the literature, observations, chemical intuition

Steric effects of nitrogen donor ligands



free bpy ligand metal complex



Free ligand Pre-organized ligand

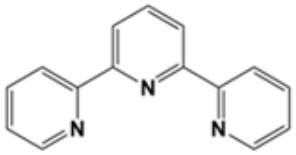
Our hypotheses:

- Preorganization → reduce kinetic binding barrier → improve efficiency
- Planarity → reduce steric repulsion between H atoms → improve efficiency
- Substitution Effects → increase electron donating group → improve efficiency

R Hancock, Chem. Soc. Rev., 2013, 42, 1500-1524

Proposed Extractants Based on the Hypothesis

Row I



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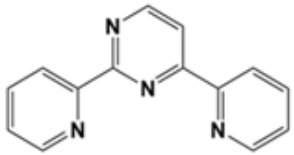

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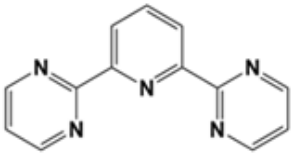

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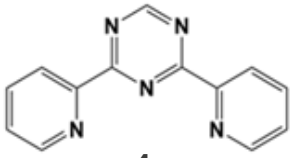

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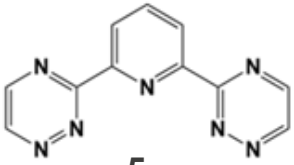

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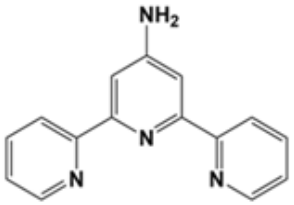
Row II



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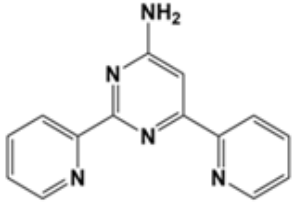

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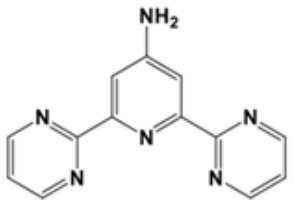

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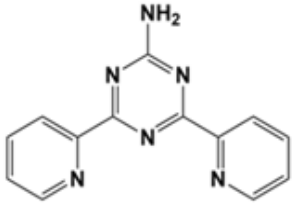

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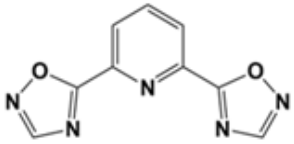
Row III



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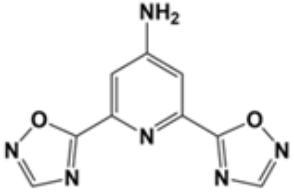

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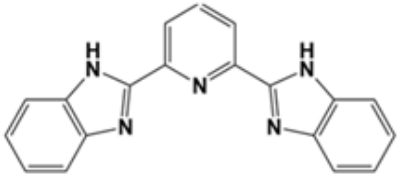

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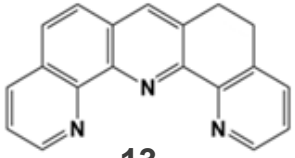
Row IV



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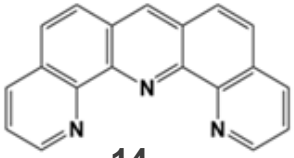

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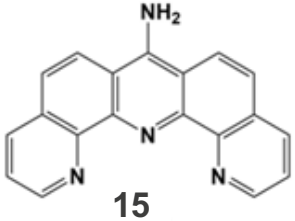
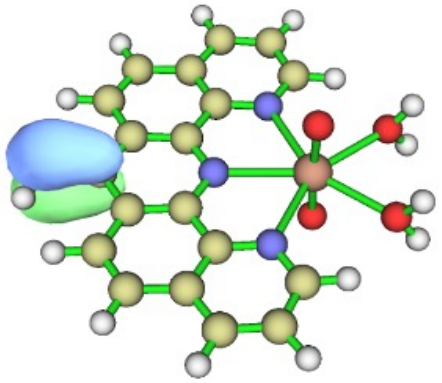
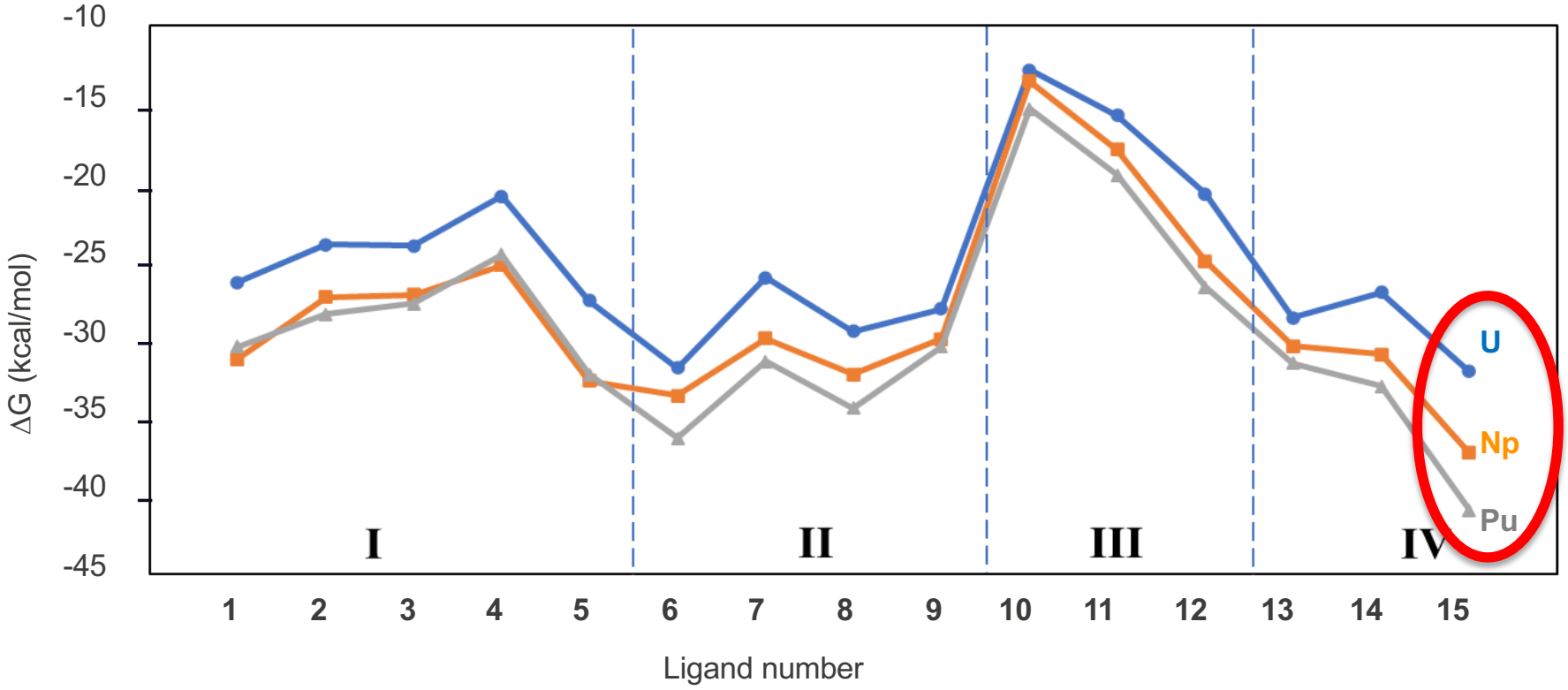


15

Construct Investigation: Binding Energies of Extractants

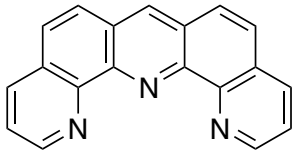
AnO_2^{2+}, An = U, Np, Pu
as model systems for the screening process.





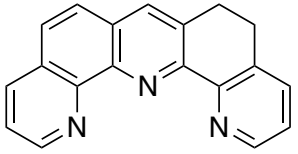
Synthesis and Separation Experimental Validation

14

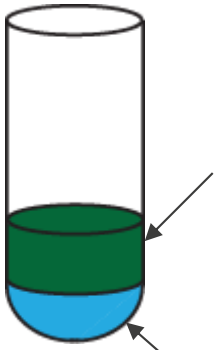


Not soluble in non-volatile organic solvents
→ not great for liquid/liquid extraction

13, dpap

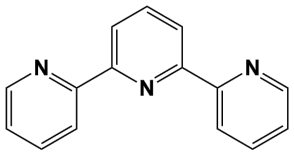


Precursor ***is soluble*** in *n*-octanol, still has the pre-organized N donors

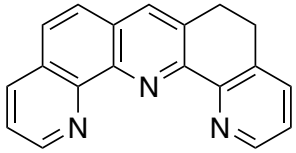


n-octanol + 20 mM "L" +
1 M 2-bromohexanoic acid

0.01 M HNO_3 +
^{241}Am and ^{155}Eu tracers



"L" = terpy

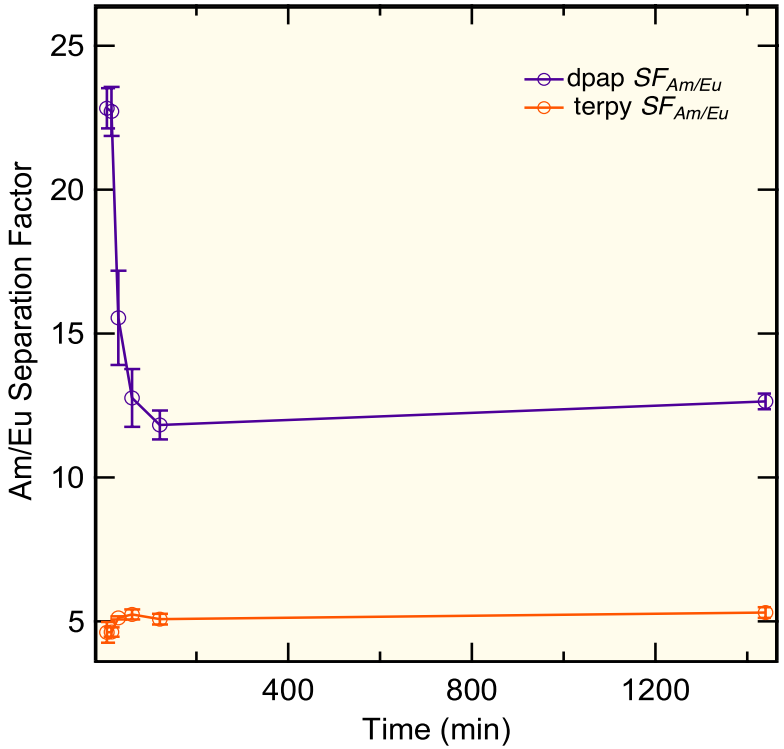


"L" = dpap

Close integration between theory and experiment is critical as cross-validation is highly needed!

X Zhang, SL Adelman, SA Kozimor, BW Stein, ER Batista, P Yang, et al ***2022,*** *61, 11556-11570*

Distribution Coefficients and Separation Factors

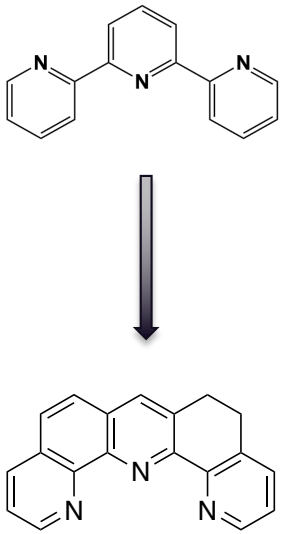


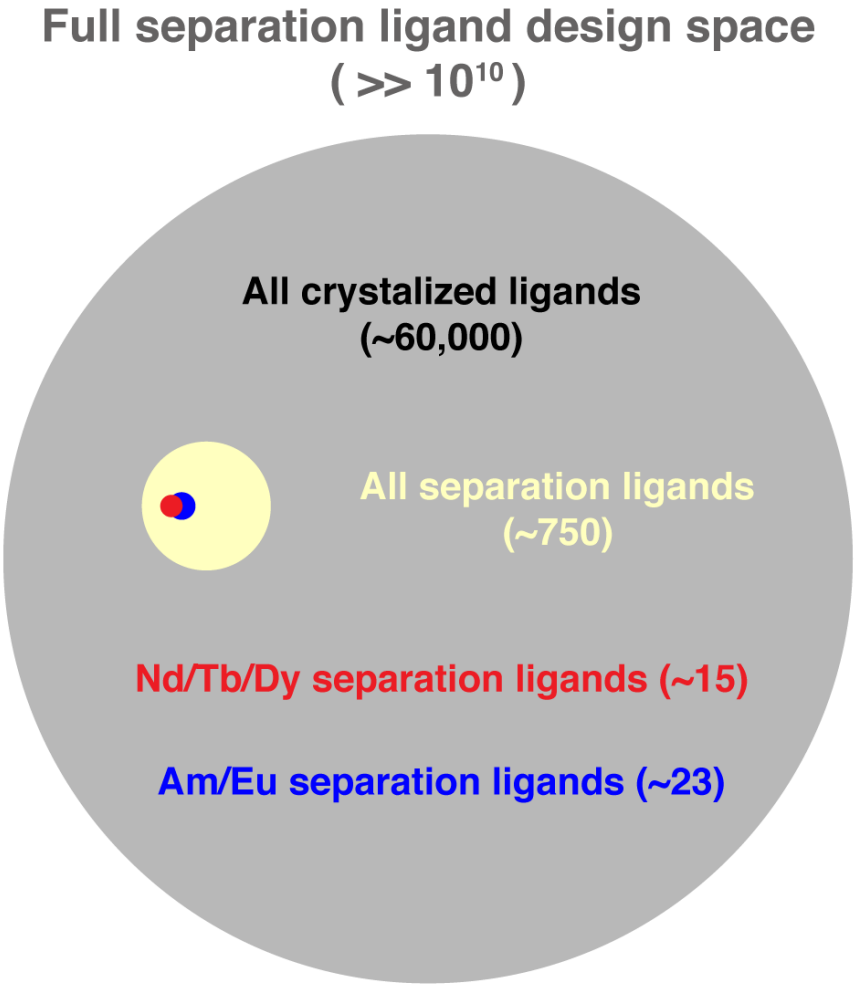
- At early times (<15 min), dpap is **~5x** better than terpy at separating Am from Eu
- Once equilibration has been reached, dpap is only **~2x** better than terpy.
- Larger separation factors with dpap are due to rapid and substantial transport of Am into organic phase
- This kind of fundamental knowledge will be used to design ligand features for the ML model

Time (min)	terpy			dpap			dpap/terpy		
-	Am D	Eu D	Am/Eu SF	Am D	Eu D	Am/Eu SF	Am D	Eu D	SF
5	0.20	0.04	4.62	12.77	0.56	23	64	13	5
15	0.25	0.05	4.63	25.59	1.13	23	101	21	5
30	0.37	0.07	5.12	16.90	1.09	16	45	15	3
60	0.39	0.07	5.24	31.73	2.49	13	82	34	2
120	0.38	0.07	5.08	30.47	3.01	10	81	40	2
1440	0.33	0.06	5.31	39.55	3.13	13	122	51	2

X Zhang, SL Adelman, SA Kozimor, BW Stein, ER Batista, P Yang, et al ***2022,*** *61, 11556-11570*

Local Exploration vs. the Vast Chemical Space



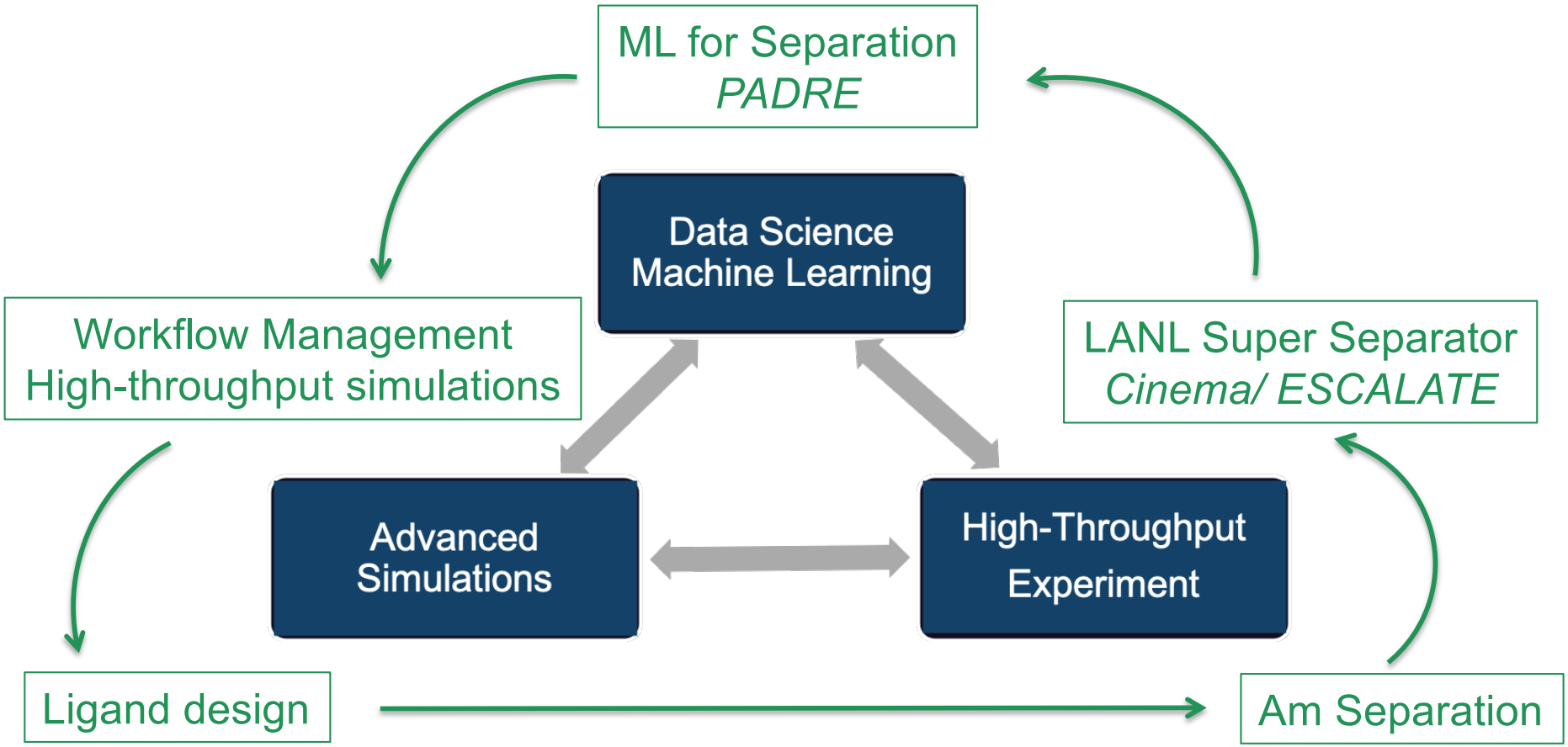


Missed chemistry

Nd/Tb/Dy 98% !

Am/Eu 97%!

Approach: SeparationML



Follow the data!

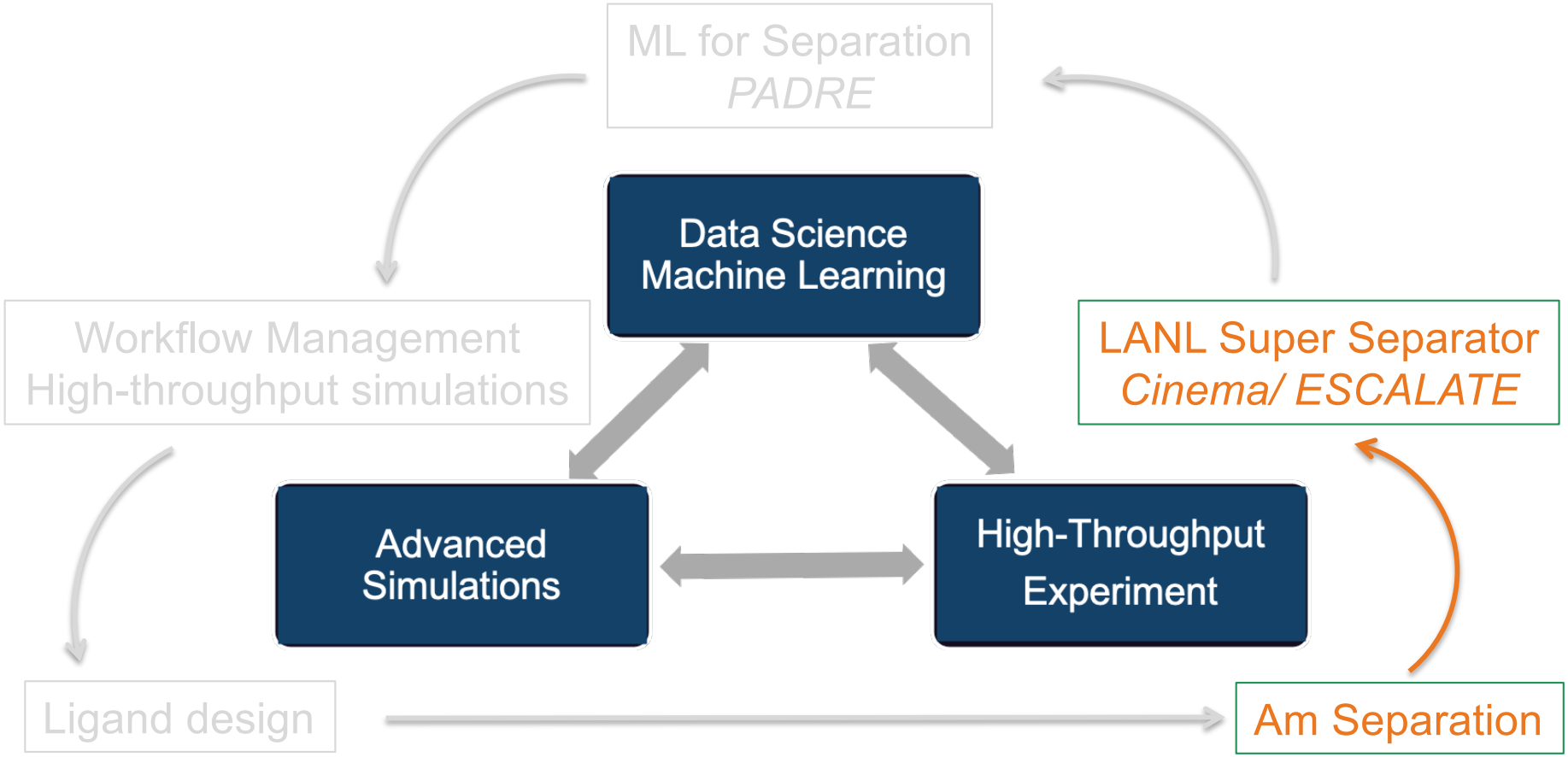
Complex workflow management is a necessity.

Challenges of Applying Data-Science for An/Ln Separation

What is Needed: Data!!!

- **High-throughput randomized uniform experimental data covering the vast chemical space.**
- **High-throughput theoretical data through advanced simulations**
  - Screen millions of ligands/extractants
  - Form chemically sensible An/Ln complexes
  - Manage thousands of calculations simultaneously
  - Quantum-based simulations for bond forming & breaking
  - Long-timescale molecular dynamics simulations across interfaces

Approach: SeparationML



Follow the data!

Complex workflow management is a necessity.

Workflow of a K_d Measurement Using Extraction Resins
(in a regular lab)

Step 2

Assay Solution

Step 3

Weigh and condition resins

Step 4

Contact resins with ^{241}Am

Step 5

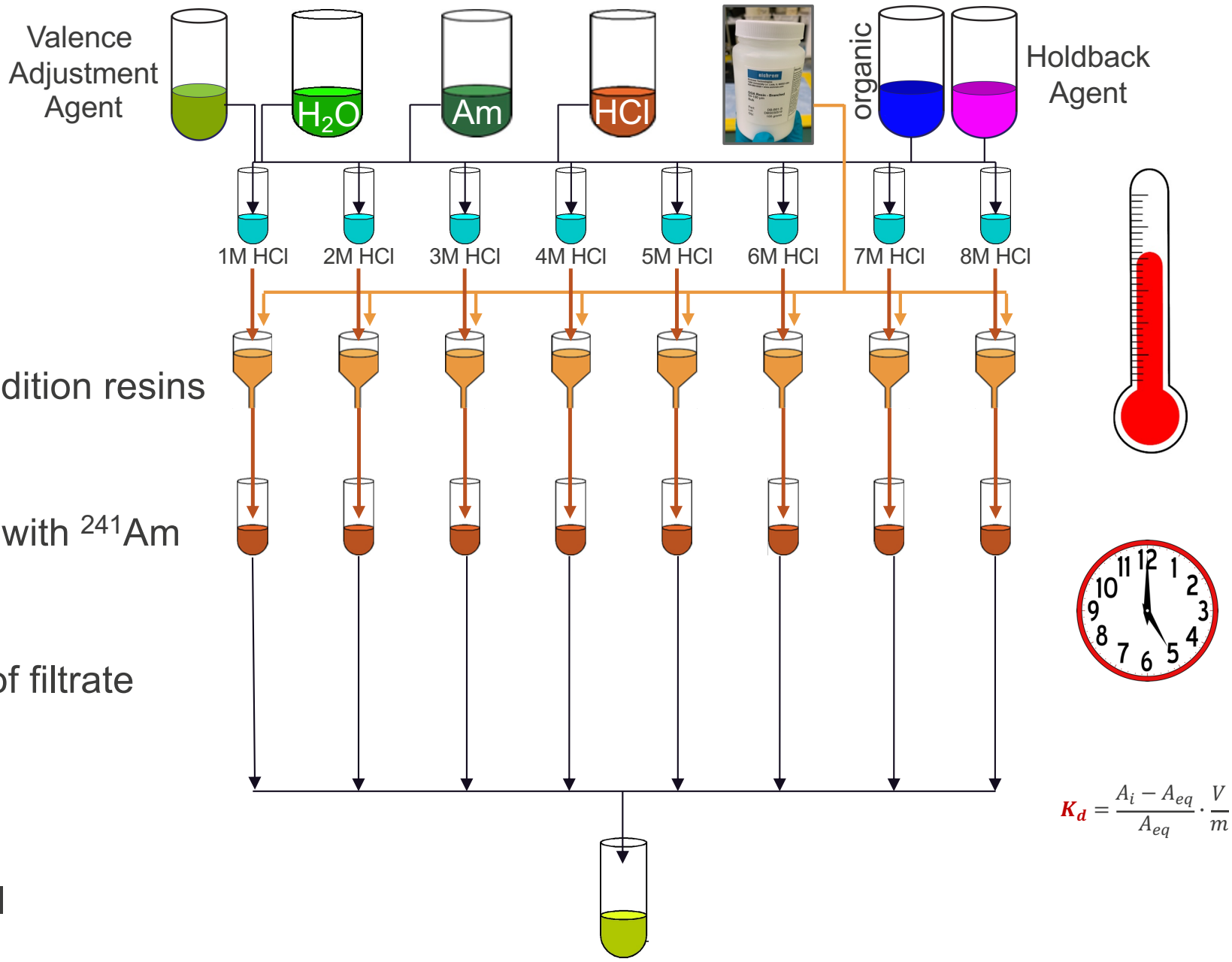
Assay Aliquot of filtrate

Step 6

Calculate K_d

Step 7

Waste disposal



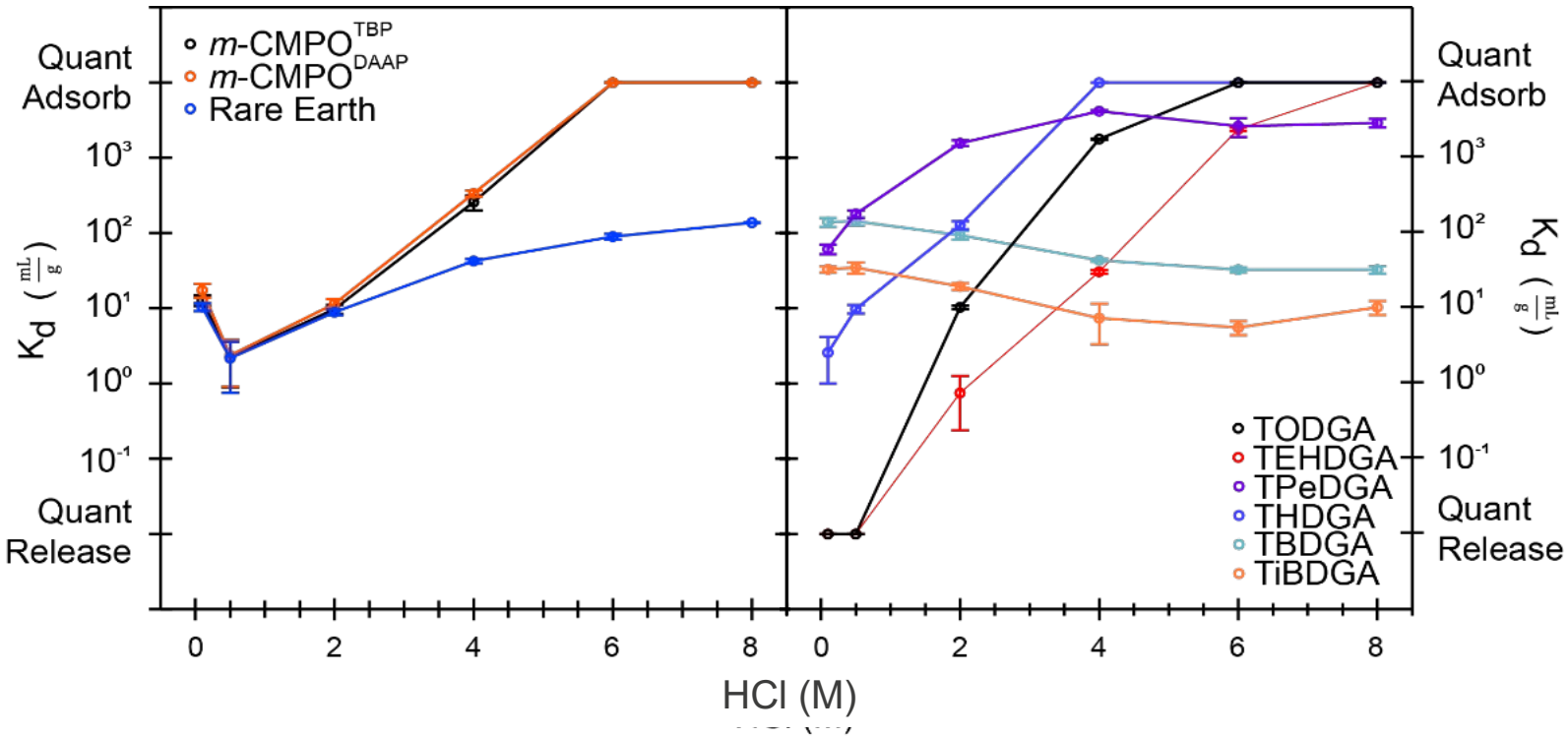
$$K_d = \frac{A_i - A_{eq}}{A_{eq}} \cdot \frac{V}{m}$$

Summary: Matrix Effects on Am Processing

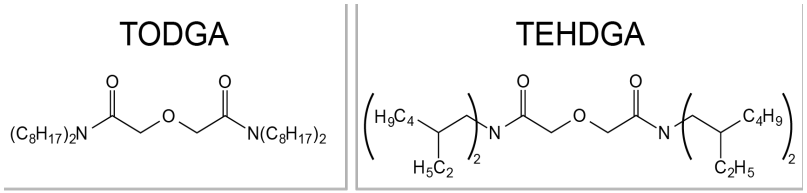
342 experiments later

Seven Tested Properties

Extractant identity	Binding capacity
Phase transfer catalysts	Bead size
Matrix effect	Binding kinetics
Aqueous matrix	

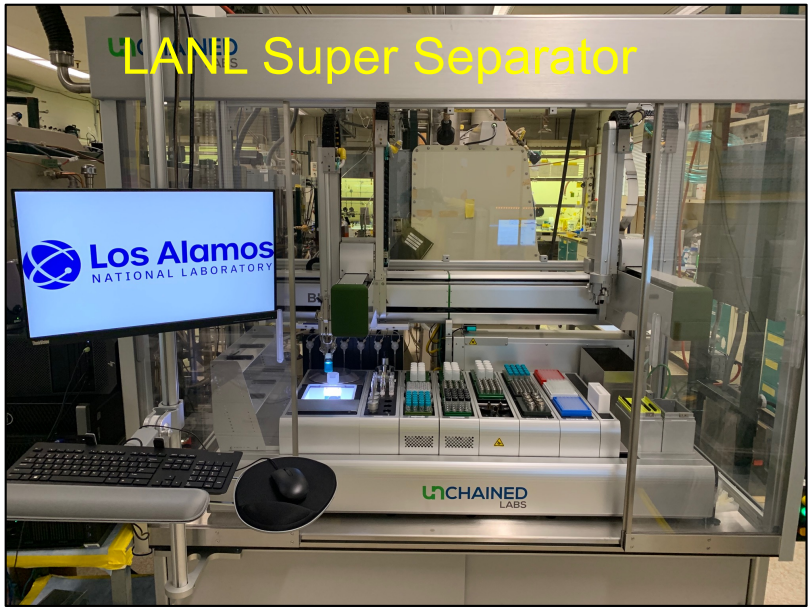


- TEHDGA and TODGA >> *m*-CMPO^{TBP} and *m*-CMPO^{DAAP} >> Rare Earth (RE) resin.
- TEHDGA and TODGA also provide a release mechanism via controlling acid concentration



BT Arko, SL Adelman, et al, Ind Eng Chem Res, ***2021***, 60, 14282–14296

Automating Separations: LANL Super Separator

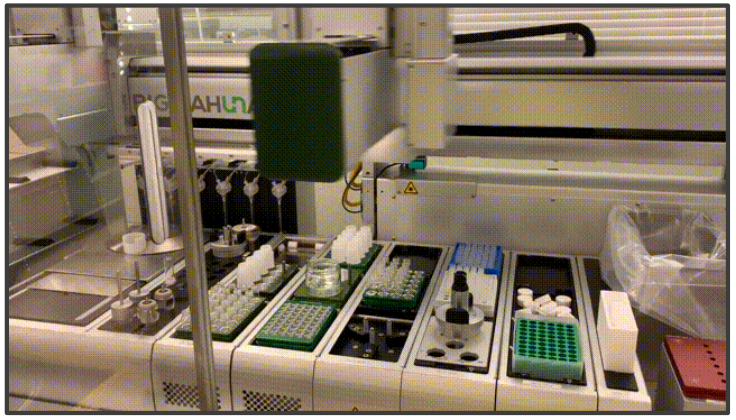


Installed in February 2021

Weighing Solids

2.0 mg of resin ± 0.2 mg

Dispensing Solutions



10 to 10000 mL of solution
with 2% to 10% error

Increases throughput

Efficient

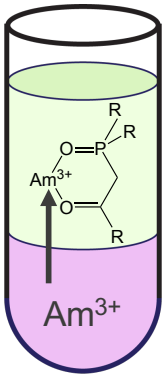
Human error

Cost Saving

- Makes it easier to develop a new process.
- Makes it easier to optimize an operational process with the confines of an existing safety envelope.

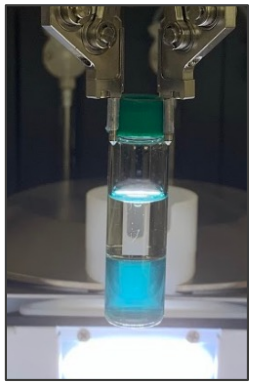
Automating Separations: LANL Super Separator

Solvent Extraction

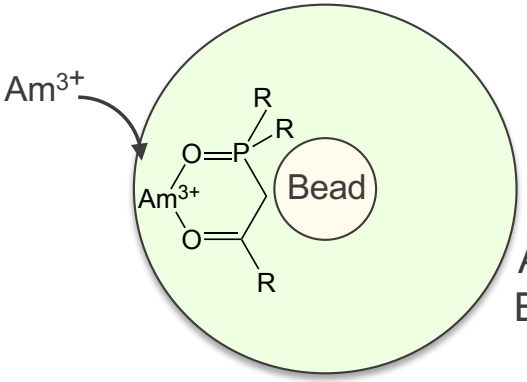


Organic Solvent

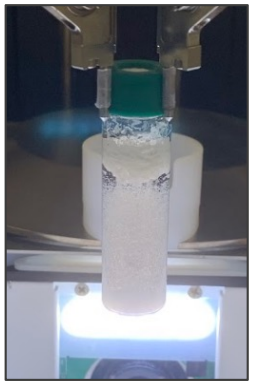
Aqueous Solution



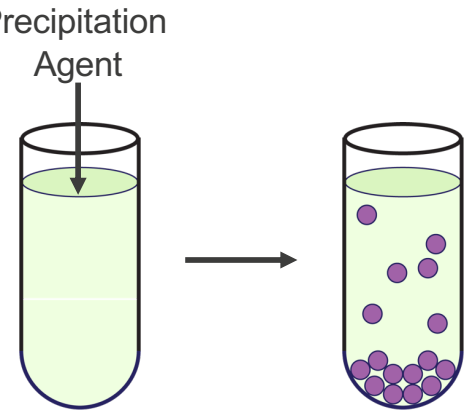
Extraction Chromatography

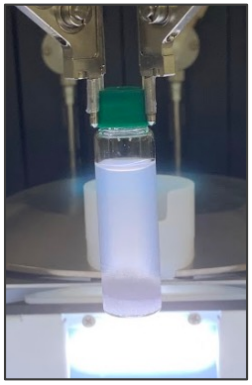


Adsorbed Extractant



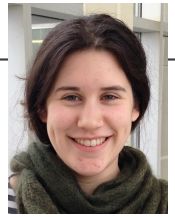
Selective Precipitation





- ~~Automation increases throughput and~~ minimizes human error.
- Commissioned U and Th; transuranics soon

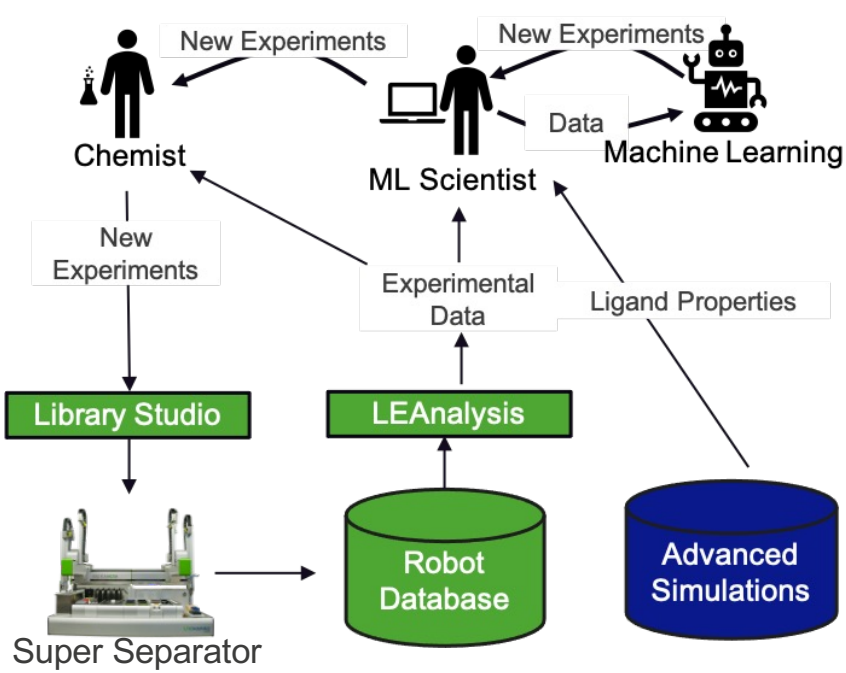
Stosh Kozimor

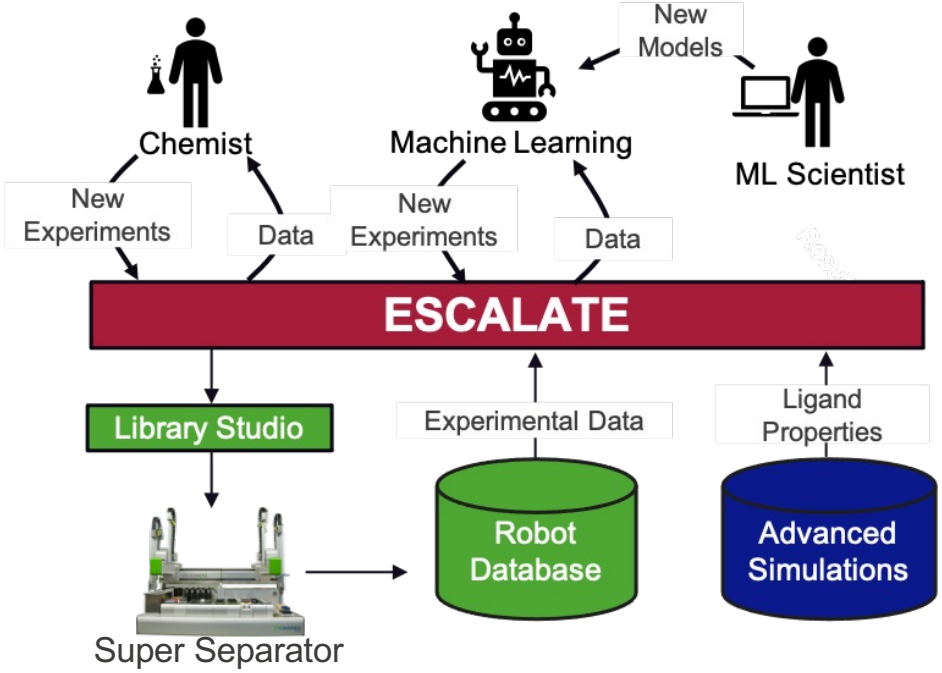


Sara Adelman

Interfacing the robot with ML: ESCALATE

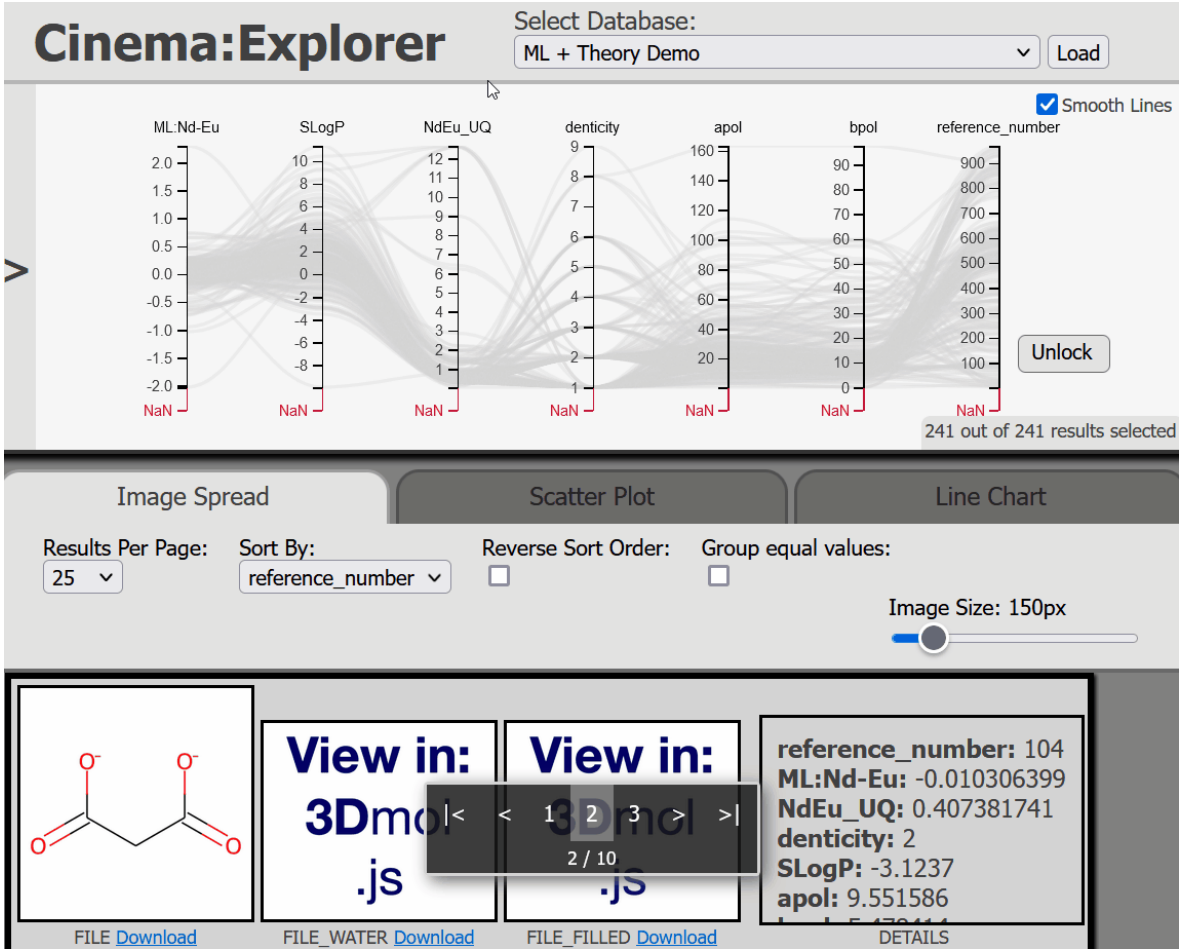
- Provides an abstraction layer between chemists + ML model with the Robot
  - Reduce complicated interaction between many pieces of software and databases
- A major software engineering task
  - Enables closed-loop interaction between ML and the Robot
    - Data from robot curated to ML model
    - API for humans or algorithms to specify new experiments
  - Enables easy visualization of large dataset through single web application





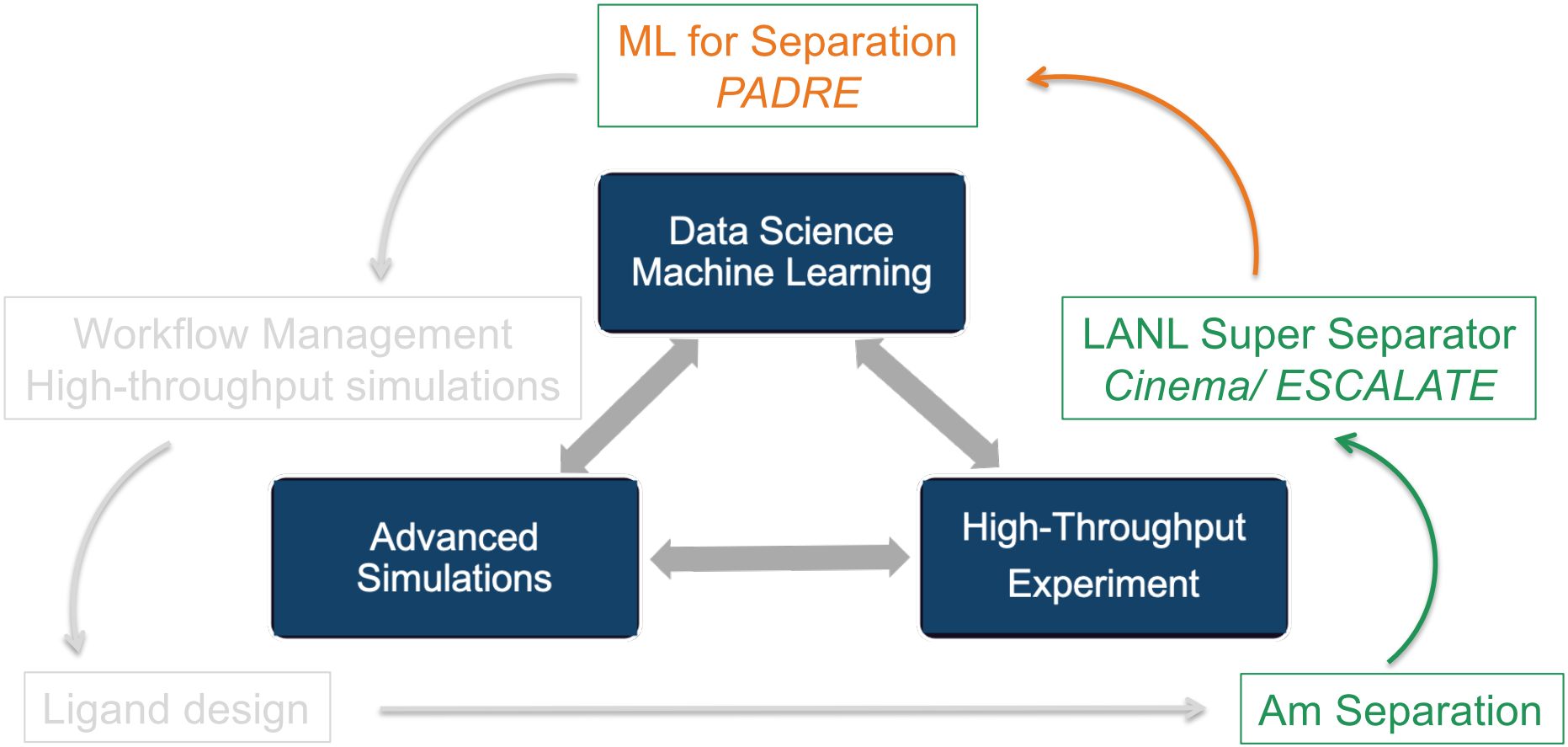
Interactive Virtualization of High-dimensional Data

- Cinema Science tool allows interactive data analysis and visualization of theory, ML, and experimental data, especially large volume and high-dimension
- 3D molecular viewer, regular expression queries, other advanced features added by SeparationML team
- Collaboration with DOE-ASCR, ECP, SciDAC programs:
  Data Science at Scale.



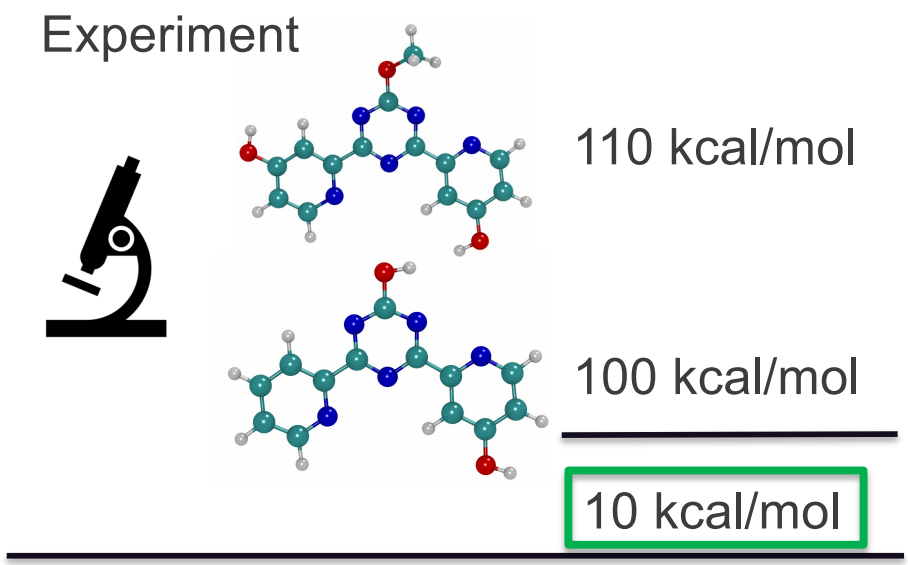
https://cinemascience.github.io/

Approach: SeparationML



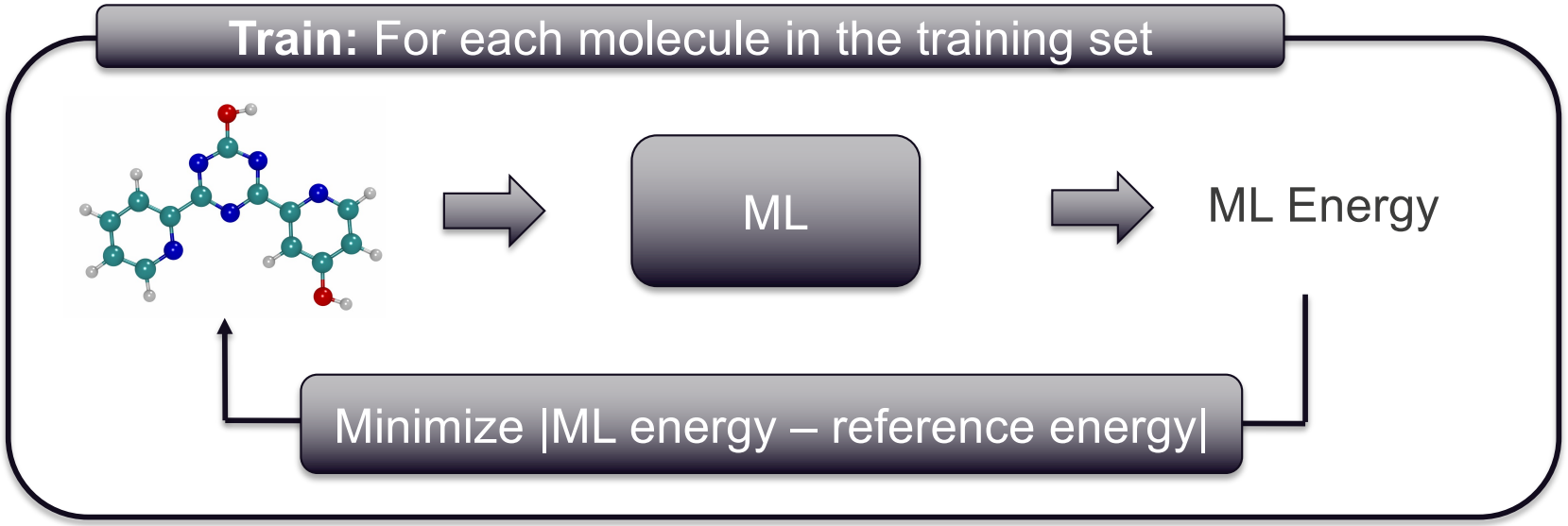
The ML Model: Motivating Observation

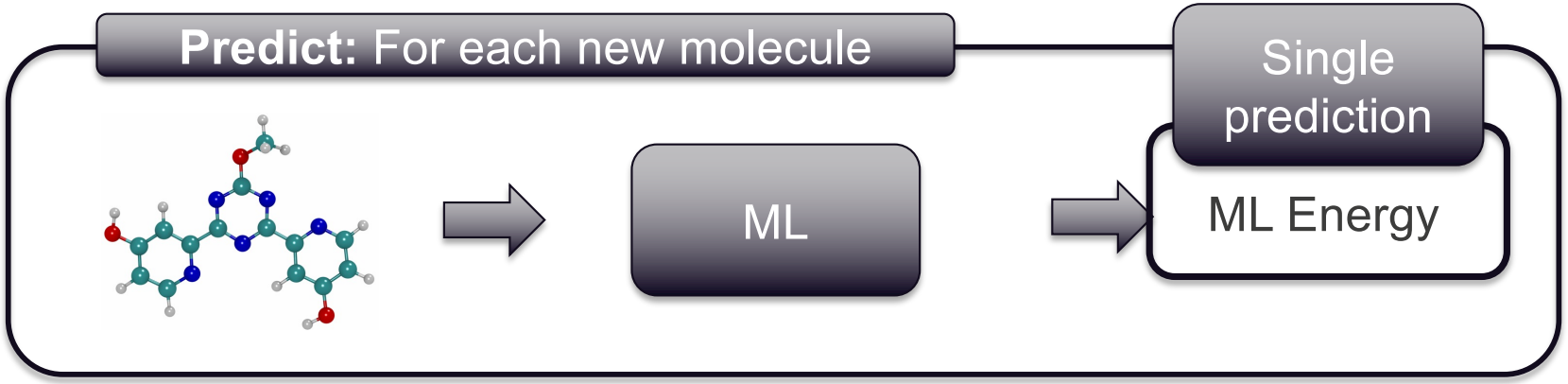
- Errors in different models often cancel: calculated energy differences are often much more precise than absolute values.
- "Chemistry informed ML": Can this be applied to the ML models as well?
- We have developed a "pairwise" ML method that addresses key challenges of:
  - uncertainty quantification
  - limited size datasets



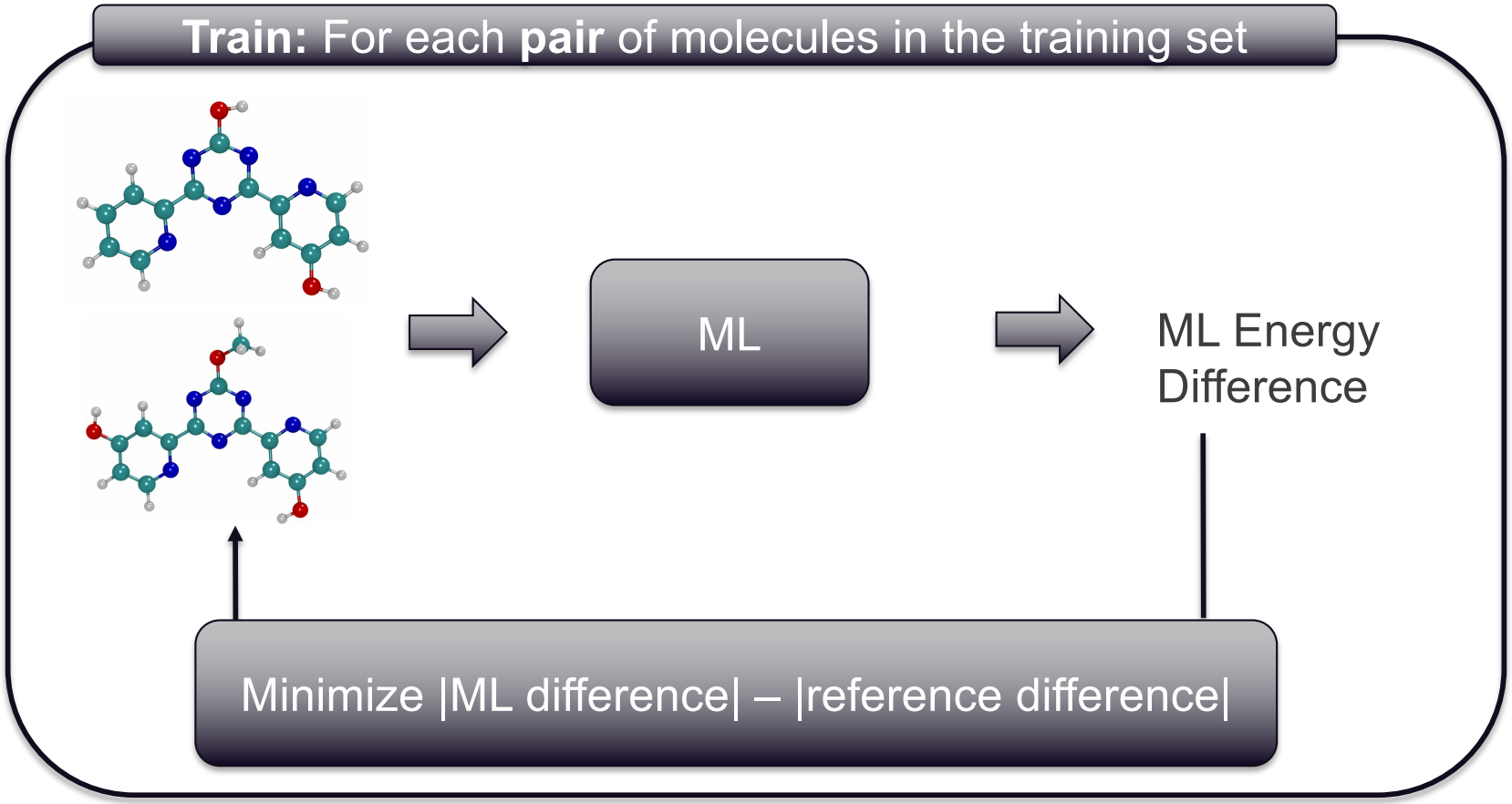
M Tynes, W Gao, DJ Burrill, ER Batista, D Perez, P Yang, N Lubbers, J. Chem. Inf. Model, ***2021****, 61, 3846-3857*

Conventional ML

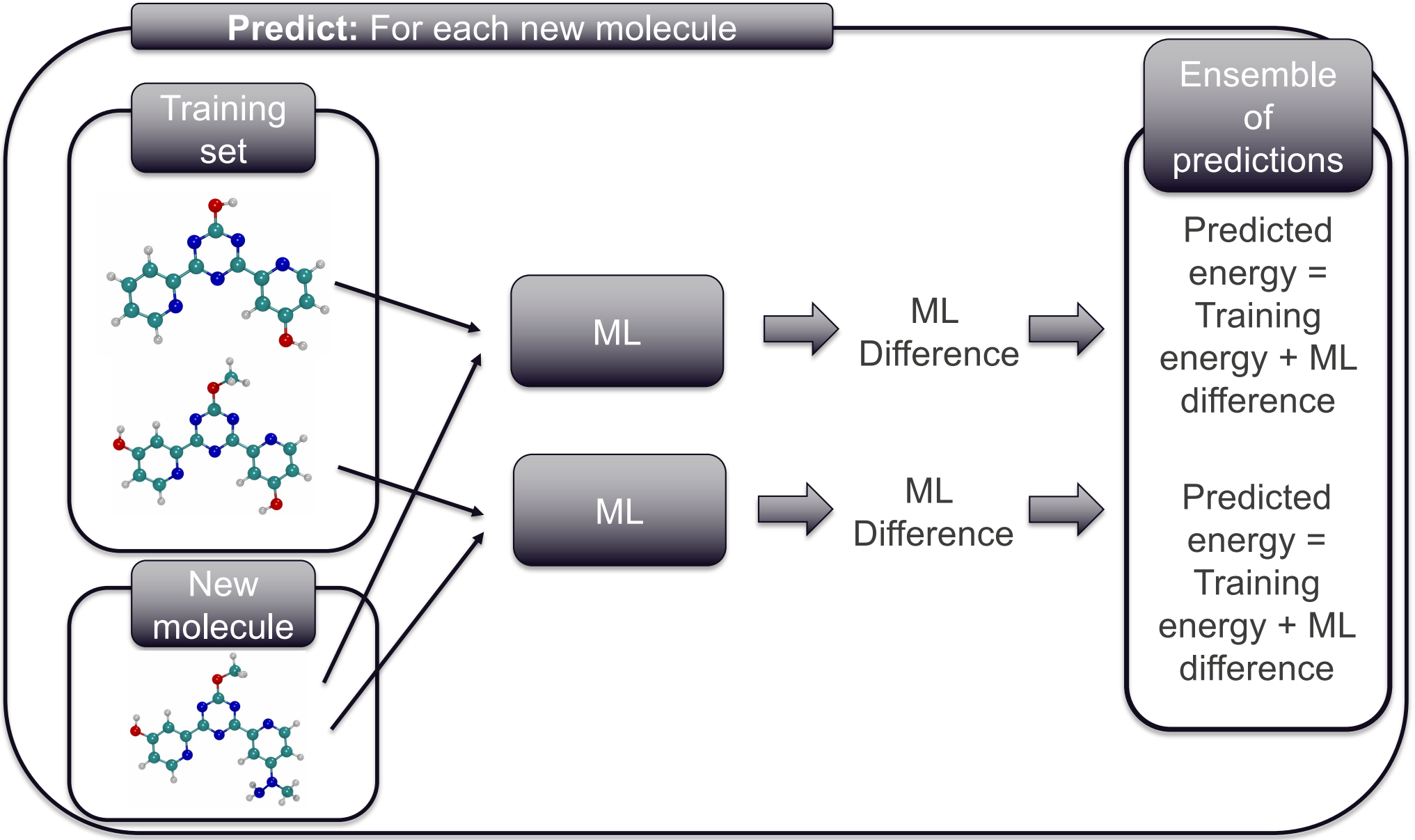




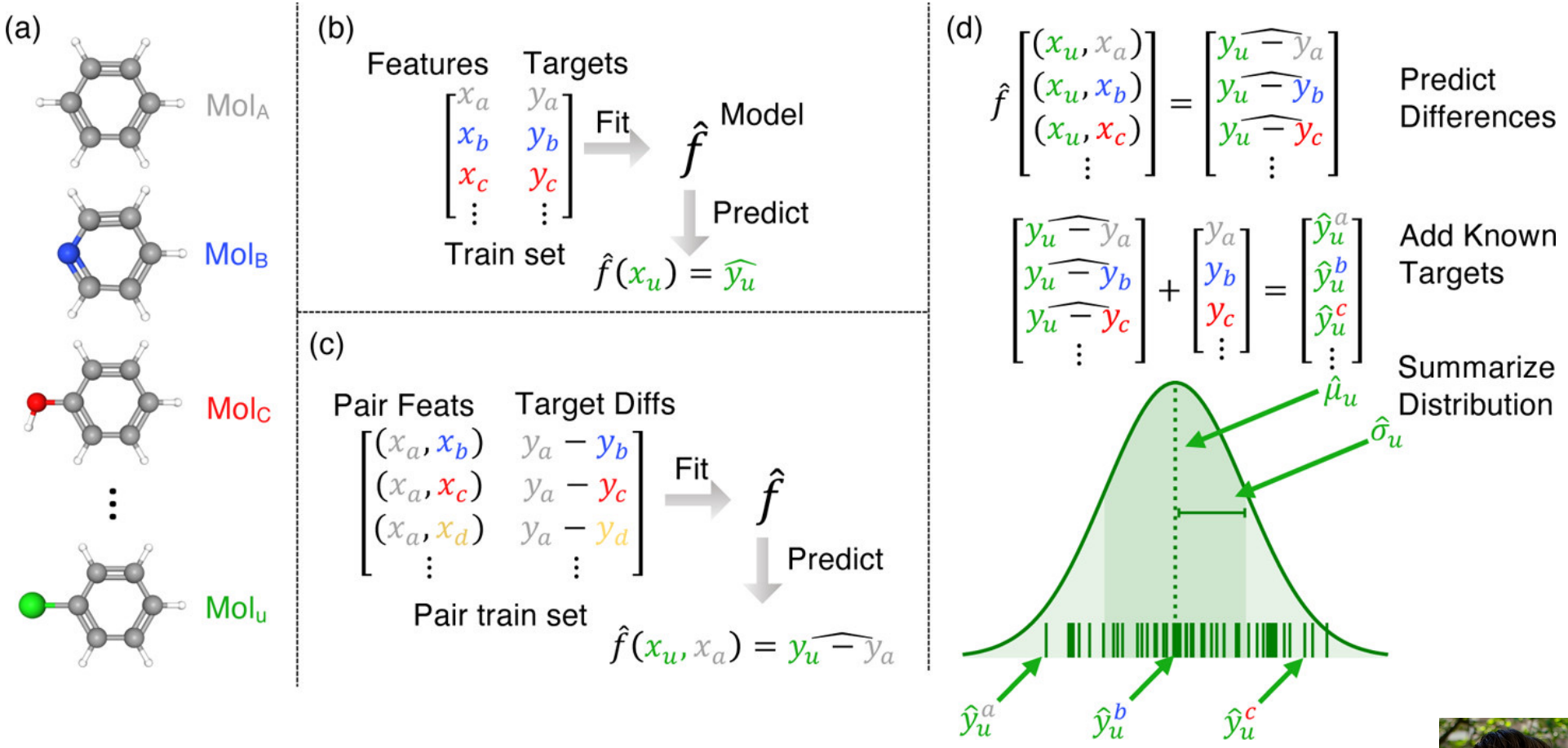
ML Model: Pairwise Difference Regression (PADRE)



ML Model: Pairwise Difference Regression (PADRE)



PADRE Algorithm Overview



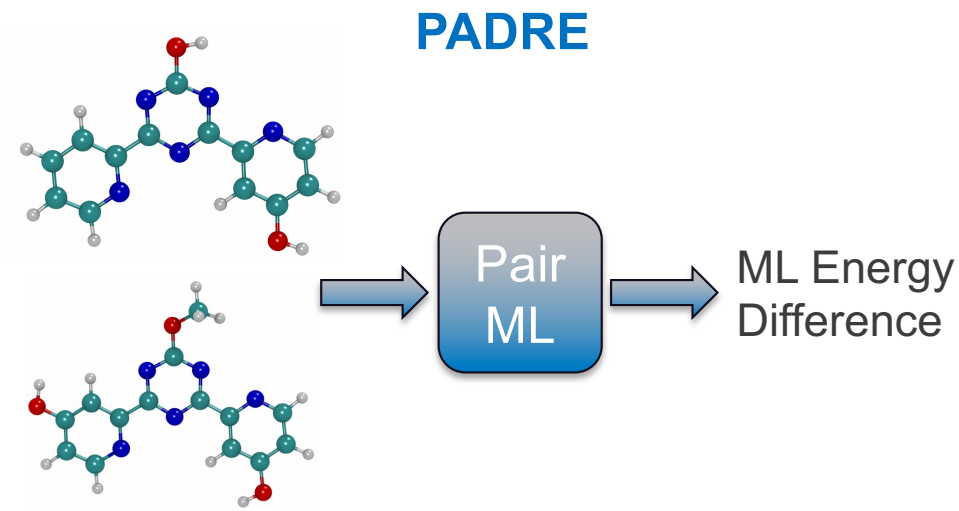
M Tynes, W Gao, DJ Burrill, ER Batista, D Perez, P Yang, N Lubbers, J. Chem. Inf. Model, ***2021****,* 61, 8, 3846–3857

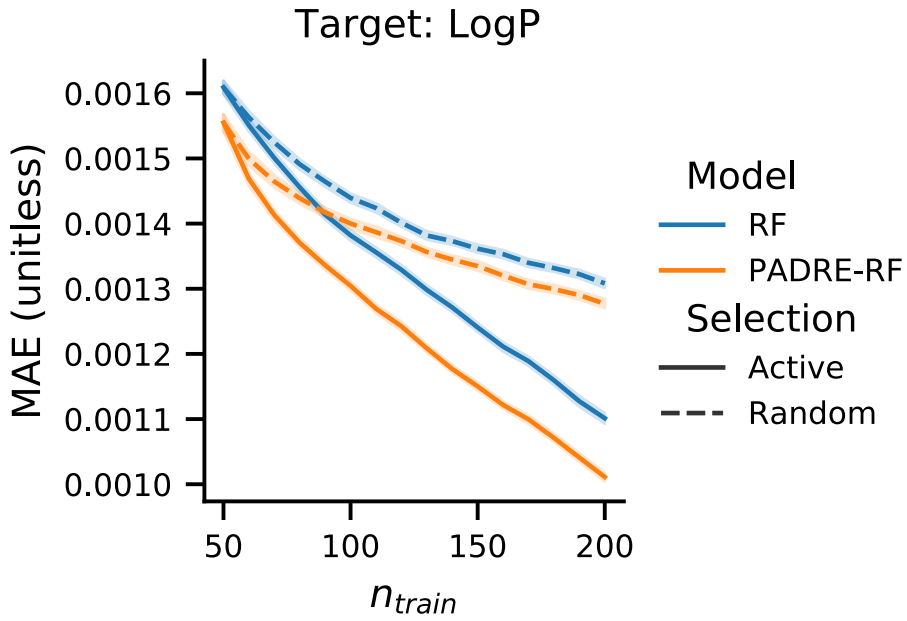
Mike Tynes

PADRE: Features & Performance

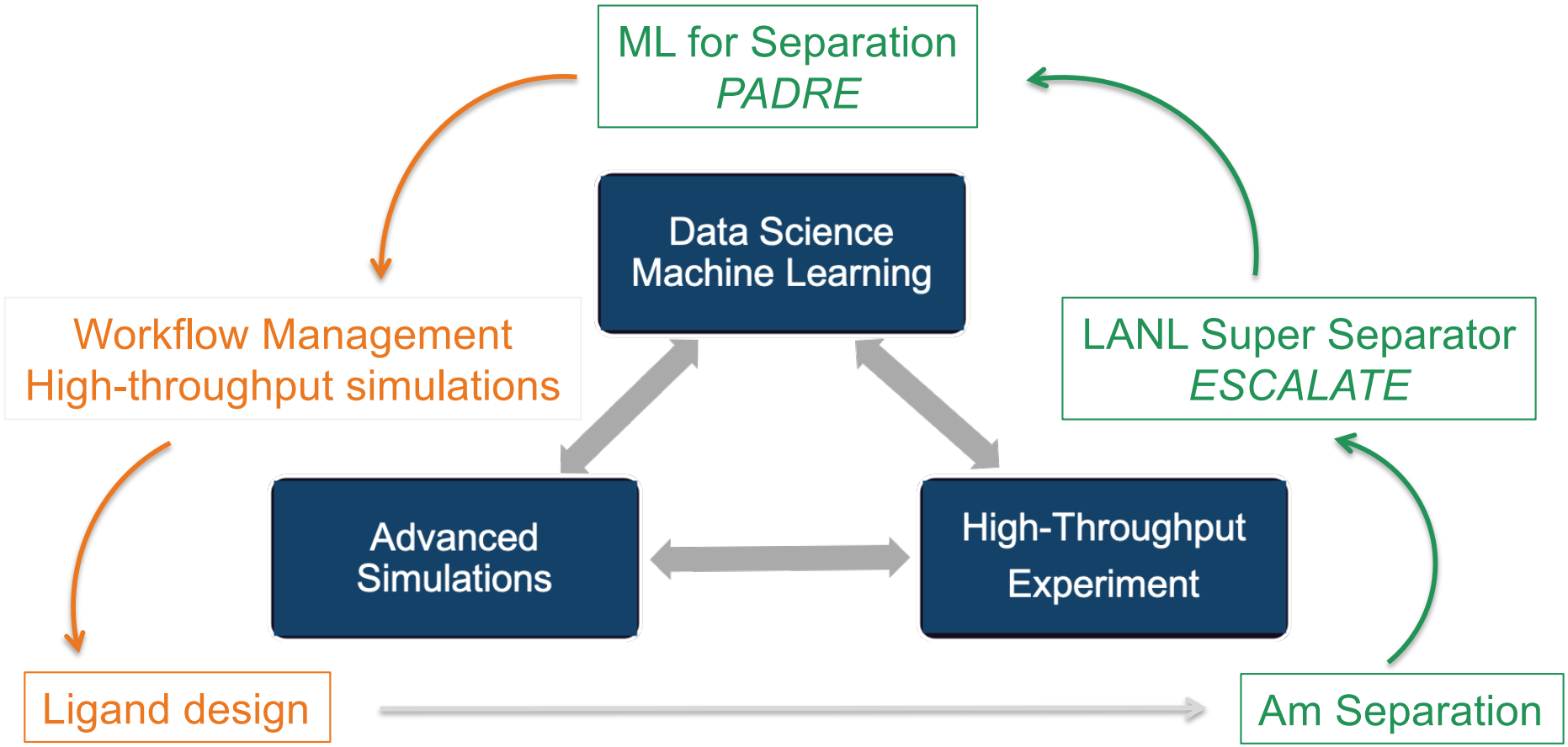
A chemistry-informed ML model
Pairwise difference regression:

- *Predict relative quantities, e.g. Separation Factors*
- n^2 data augmentation
  - Train on all pairs
  - Improve prediction by 10%
- ML meta-algorithms for arbitrary base regressors
  - Simple RF+PADRE is competitive with more complex NN
  - Redox, solubility, and BE
- Provides a useful UQ metric
  - Competitive with state-of-the-art chemical candidate selection



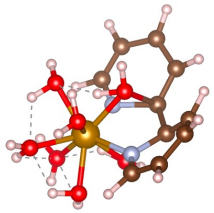


Approach: SeparationML

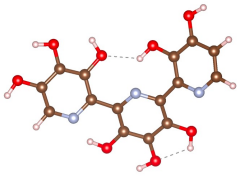


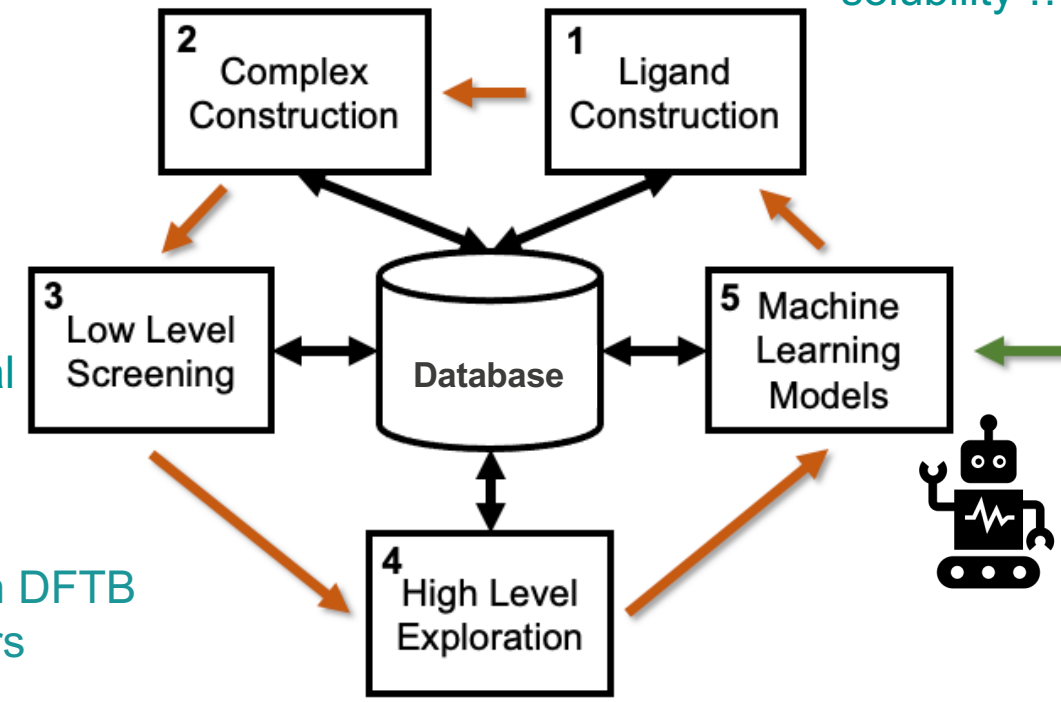
High-throughput Quantum Simulations

Architector, Generate chemically-sensible extractant-actinide complexes



Vulcan, Suggest new extractants factoring in synthesizability, pH, solubility …





ESCALATE, improved for separation science

Mineva, calculate topological chemical descriptors

EPO, train DFTB parameters

ADF/Gaussian, DFT calculations

pyiron, complex workflow management package for all-level calculations simultaneously using HPC to enable automatous discovery

Calculating Separation Factors

$$M^{3+}_{(aq)} + 3NO^{-}_{3(aq)} + nL_{(org)} \xrightarrow{\Delta G_{ext}} M(NO_3)_3(L)_{n(org)}$$

$$An^{3+}_{(aq)} + Ln(NO_3)_3(L)_{n(org)} \xrightarrow{\Delta\Delta G_{ext}} Ln^{3+}_{(aq)} + An(NO_3)_3(L)_{n(org)}$$

$$SF_{An/Ln} = D_{An}/D_{Ln} = \exp(-\Delta\Delta G_{ext}/RT)$$

$$An^{3+}_{(aq)} + 3NO_3^-{}_{(aq)} + nL^b_{(org)} \xrightarrow{\Delta G_{ext}} An(NO_3)_3(L^b)_{n\ (org)}$$

$$- \left(An^{3+}_{(aq)} + 3NO_3^-{}_{(aq)} + nL^a_{(org)} \xrightarrow{\Delta G_{ext}} An(NO_3)_3(L^a)_{n\ (org)} \right)$$

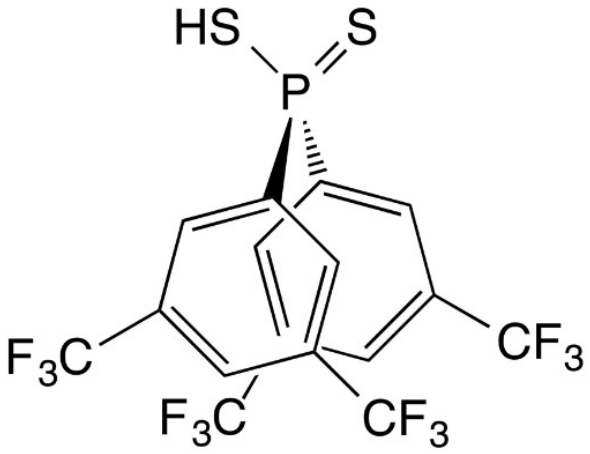
$$+ \left(Ln^{3+}_{(aq)} + 3NO_3^-{}_{(aq)} + nL^a_{(org)} \xrightarrow{\Delta G_{ext}} Ln(NO_3)_3(L^a)_{n\ (org)} \right)$$

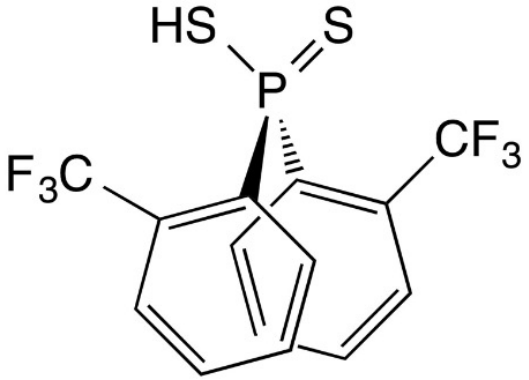
$$- \left(Ln^{3+}_{(aq)} + 3NO_3^-{}_{(aq)} + nL^b_{(org)} \xrightarrow{\Delta G_{ext}} Ln(NO_3)_3(L^b)_{n\ (org)} \right)$$

$$An(NO_3)_3(L^a)_{n\ (org)} + Ln(NO_3)_3(L^b)_{n\ (org)} \xrightarrow{\Delta\Delta\Delta G_{ext}} Ln(NO_3)_3(L^a)_{n\ (org)} + An(NO_3)_3(L^b)_{n\ (org)}$$

JM Keith, ER Batista, *Inorg Chem* **51,** 13–15 (2012). AE Clark, P Yang, JC Shafer, in *Experimental and Theoretical Approaches to Actinide Chemistry* 2018, pp 237-282 ; AE Clark, MJ Service, et al, *Ion Exchange and Solvent Extraction, Vol 23, 147, 2019*

An Example of Calculating Separation Factors





	L1		L2	
$SF_{Am/Eu}$	20		100,000	
$\Delta\Delta G_{ext}$	–1.8		–6.8	
$\Delta\Delta\Delta G_{ext}$		–5.0		kcal/mol

JM Keith, ER Batista, *Inorg Chem* **51,** 13–15 (2012). AE Clark, P Yang, JC Shafer, in *Experimental and Theoretical Approaches to Actinide Chemistry* 2018, pp 237-282 ; AE Clark, MJ Service, et al, *Ion Exchange and Solvent Extraction, Vol 23, 147, 2019*

Workflow for Calculating Separation Factors

New extractants

↓

Architector build complexes

↓

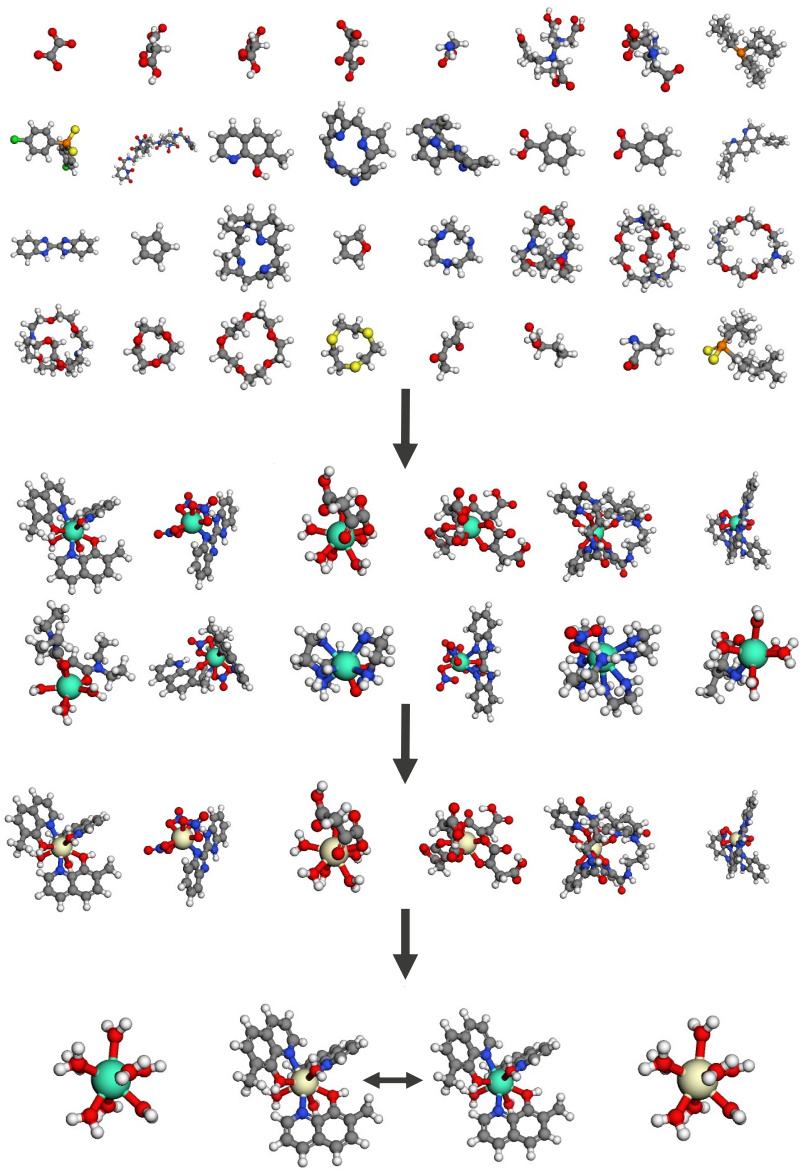
pyiron/ADF to DFT-relax 5-lowest GFN2-xTB conformers

↓

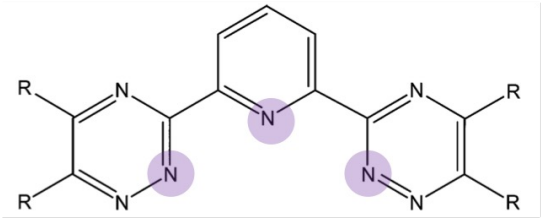
Swap Metal for other Metals + Re-optimize

↓

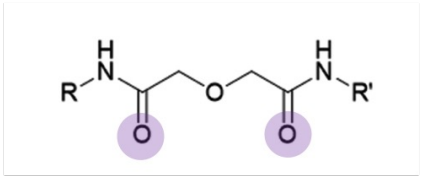
Calculate $\Delta\Delta G_{rxn}$ Swapping Metals/Ligands



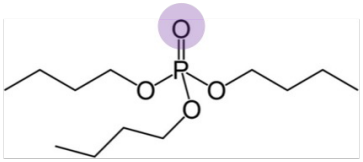
A Must: Building Chemically Sensible 3D Structures of f-Element Complexes



Bis-triazinyl-pyrine ligands (BTP)

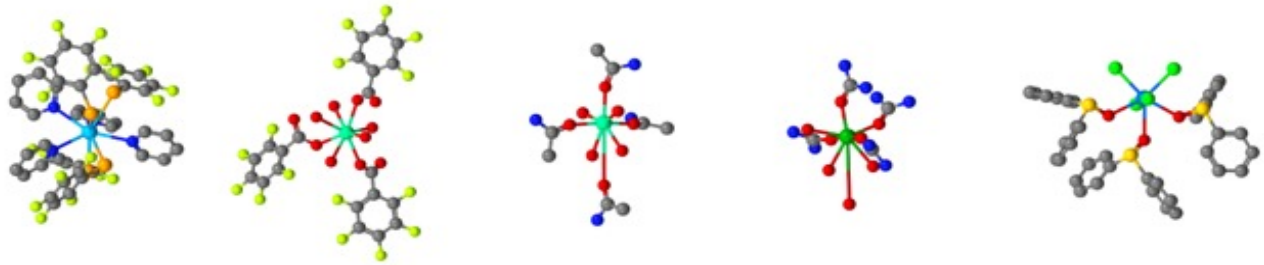


Diglycolamide (DGA)



Tributyl-phosphate (TBP)

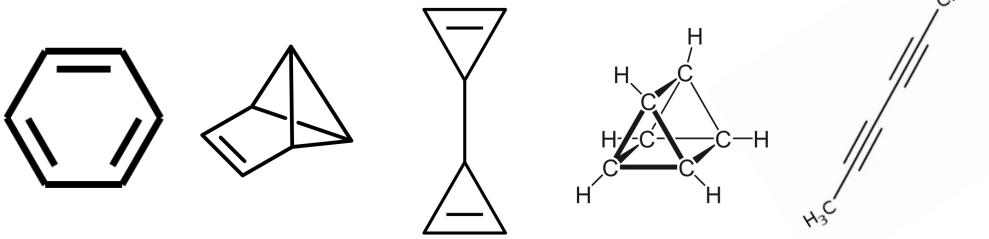
How to form 3D structures as a function of ligands, metal, coordination number, counter ions?



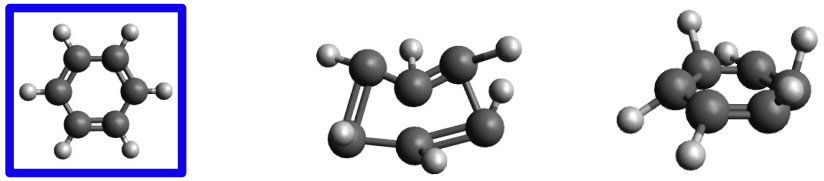
Generating 3D Structure In Chemistry

- **Degrees of abstraction in chemistry:**
  - 1D = Chemical Formula
  - 2D = Molecular Graph
  - 3D = Atomic Positions
    (Electronic Structure!)

C_6H_6

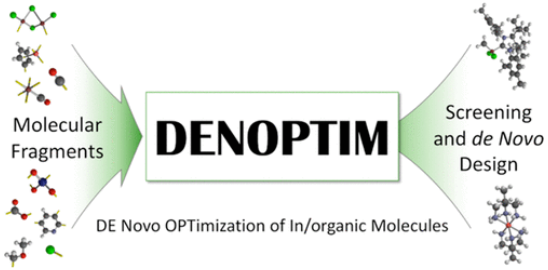


- **Moving from 3D->1D = relatively easy**
- **Moving from 1D->3D = much harder!**
- **2D -> 3D complexity alone is NP-hard**



- **d-block: molsimplify, DENOPTIM, Molassembler**
- **f-block: no tools available**

molSimplify



Molassembler

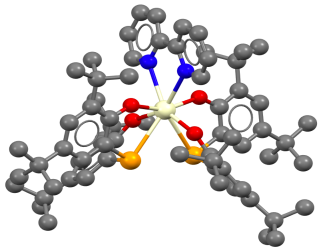
1 Thomassen, C. Journal of Algorithms 10, 568-576 (1989).

Architector Design Overview

Inputs

Metal, Coordination Number, Ligands, Coordinating atoms (CAs)

Example: Cambridge Structural Database Refcode = CONPEC

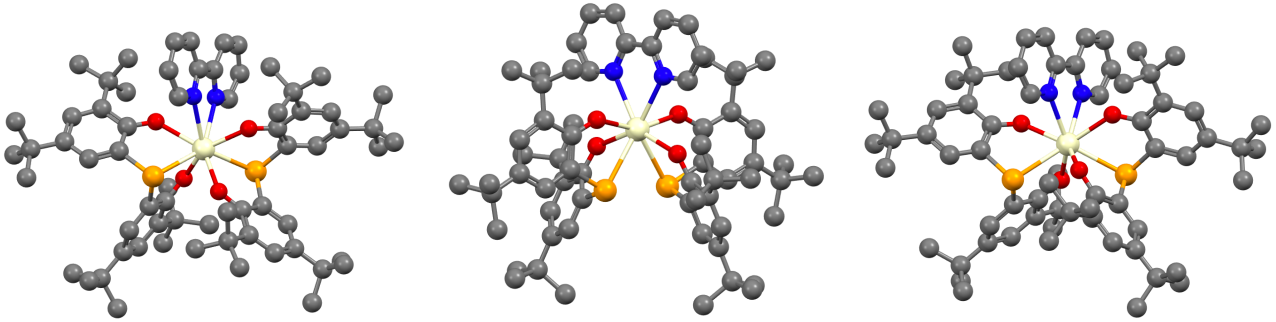


Metal: Ce
Coordination Number: 8
Ligands (SMILES, CAs):
1. c1ccc(nc1)c1ccccn1, (4, 11)
2. CC(C)(C)c1cc([Se]c2cc(cc(c2[O-])C(C)(C)C)C(C)(C)C)c([O-])c(c1)C(C)(C)C, (7,14,24) (x2)

User interactions

Outputs

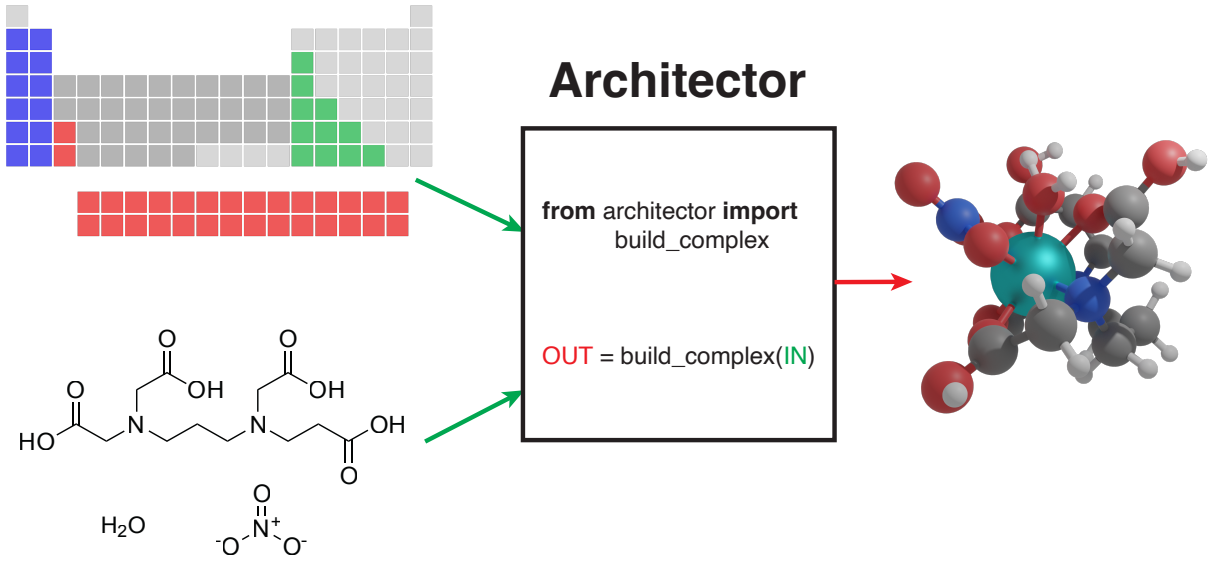
Ranked-order (by GFN2-xTB energy) complexes



Michael Taylor

https://github.com/lanl/Architector

Architector – 3D Molecule Generation Workflow



Iterate over Metal Center Symmetries

Input Chemistry → Metal Center Library/ Ligand-Metal Mapping → Generate Ligand Conformers → Assemble /Relax Complexes → Remove Duplicates → Output Structures

Computational Tools Needed for the Architector Workflow

Python:
Input/Output
Dictionary / YAML
Handles Connections
Between Software

Architector

```
from architector import
    build_complex

OUT = build_complex(IN)
```

Atomic Simulation Environment:
1. Non-forcefield Calculations
2. Structural Data

OpenBabel:
1. SMILES Conversion including charge handling
2. Ligand initial conformer generation
3. Forcefield Relaxations

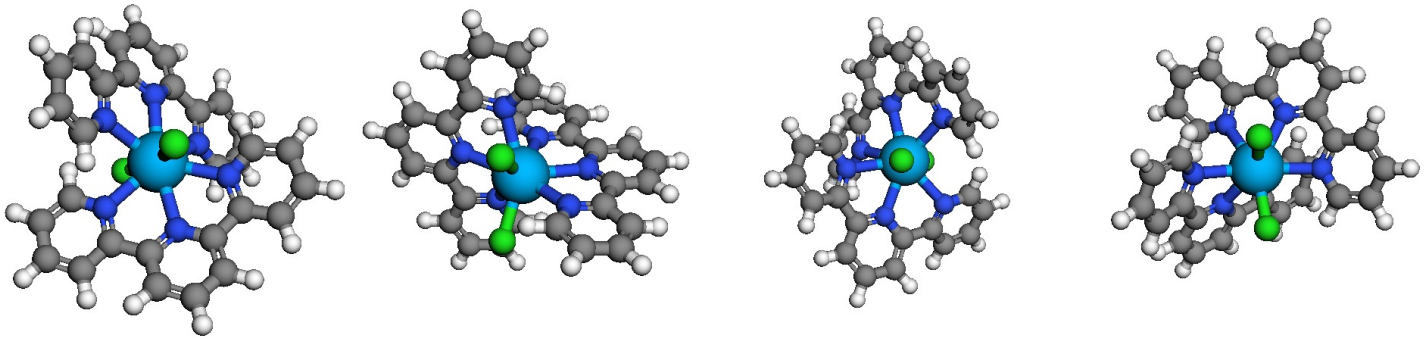
Extended Tight Binding:
1. Tight Binding Calculations
2. GFN- Forcefield Calculations

Architector Visualization

```
In [1]: from architector import build_complex,view_structures

In [3]: out = build_complex({'core':{'metal':'Th','coreCN':8},
                             'ligands':['terpy']*2+['chloride']*2,
                             'parameters':{'metal_ox':4}})

In [4]: view_structures(out)
```

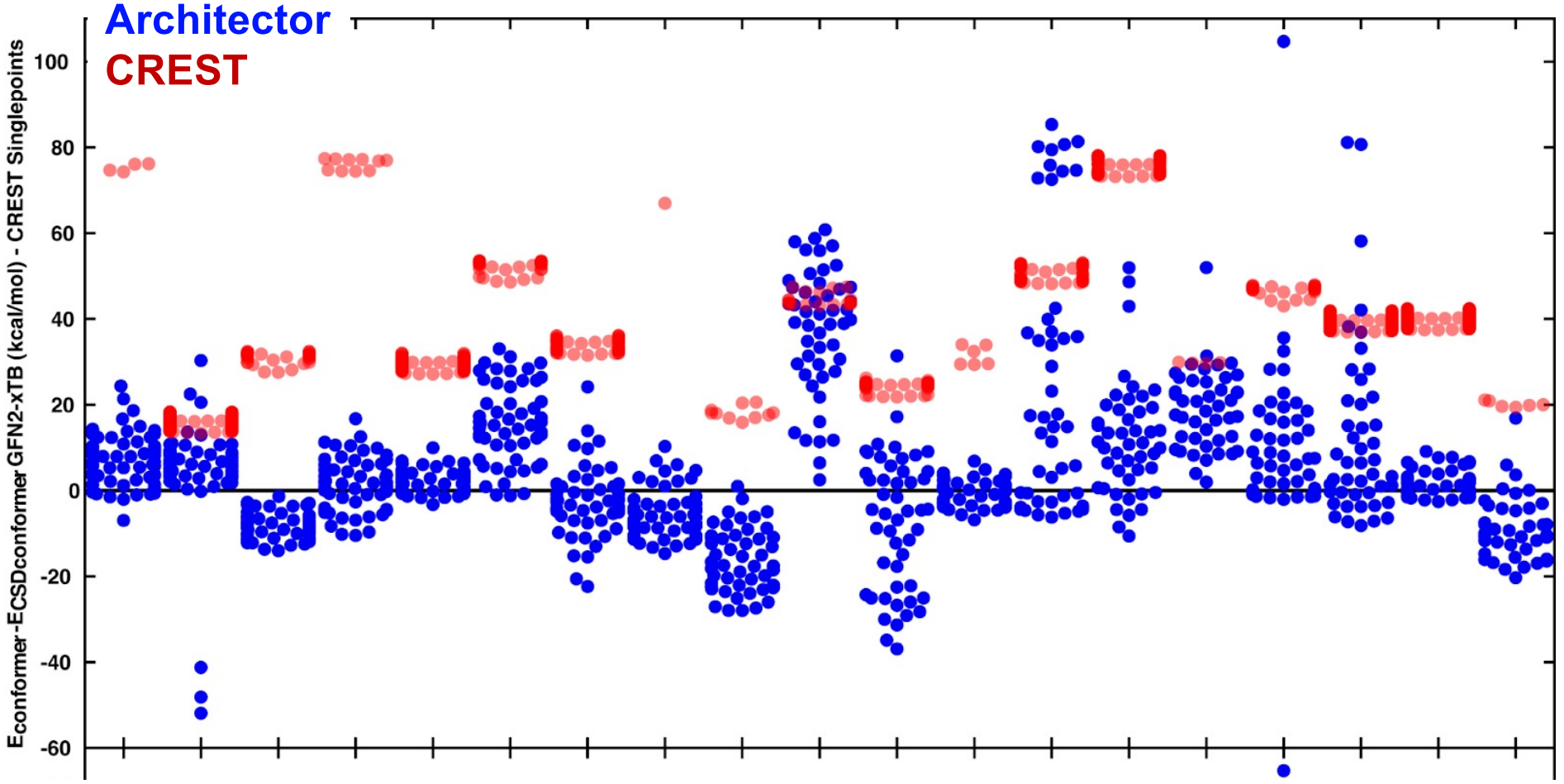


- Visualization routine integrated with jupyter notebooks – broad use-cases for visualization (dynamic grid visualization)

3Dmol.js

https://github.com/lanl/Architector

Finding New Conformers Beyond CSD Database

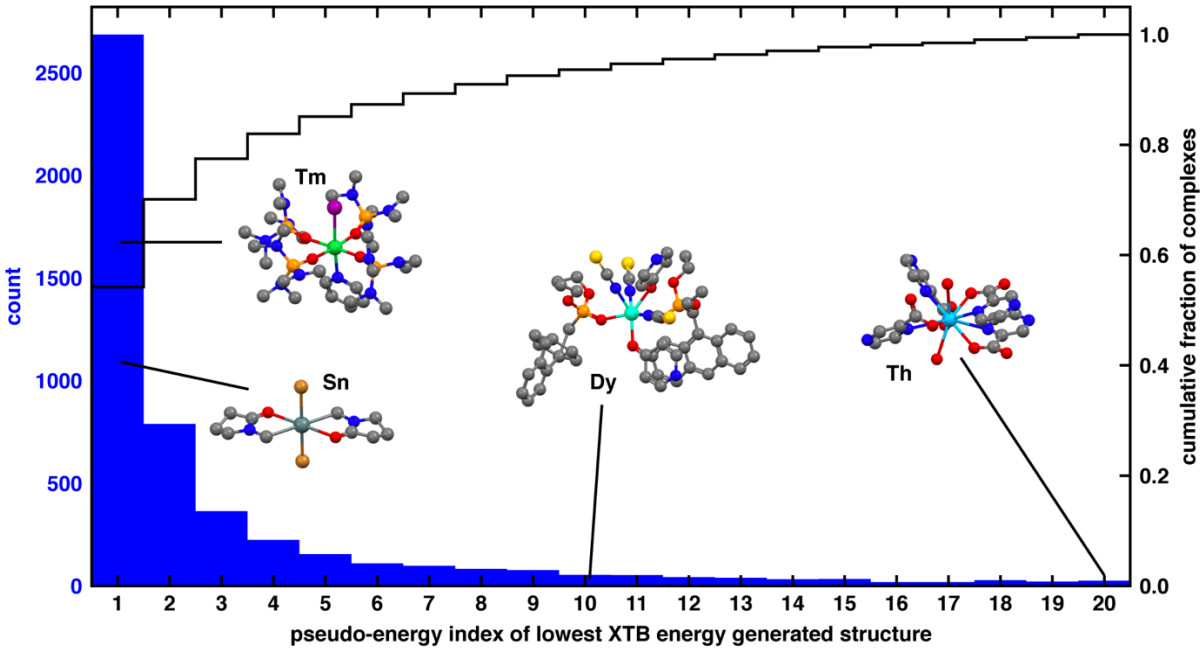


- Gas phase or liquid phase conformers can dramatically differ from crystalized structures. Conformer sampling can be vital.
- CREST[1] needs 3D structure as input, vs. Architector only needs 2D input

[1] P Pracht, F Bohle, S Grimme, *Phys Chem Chem Phys*, 2020, 22, 7169-7192

Architector Performance

- Benchmarked on over 6,500 experimental structures.
- “Embarassingly parallel” 99% finished in under 12 hours on 500 cores.
- Vast majority (95%) produced at least one conformer within 10 kcal/mol or lower than experimental structures.
- Diverse conformer generation for higher-energy symmetries.



https://github.com/lanl/Architector

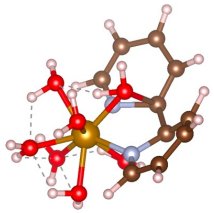
conda install -c conda-forge architector

Browser-based webserver for the community is coming. –Based on NERSC SPIN

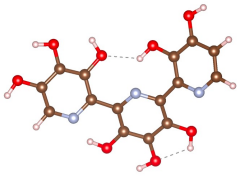
Spin

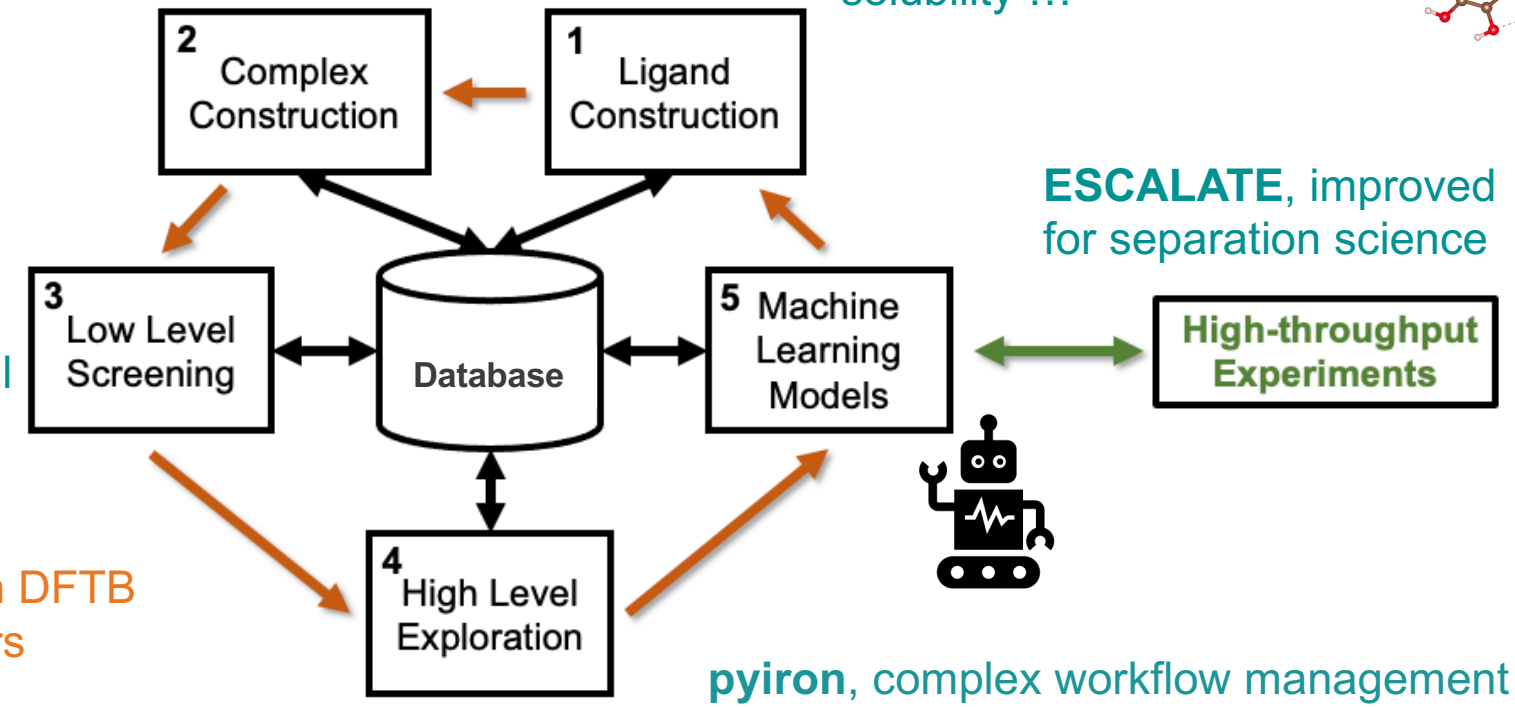
High-throughput Quantum Simulations

Architector, Generate chemically-sensible extractant-actinide complexes



Vulcan, Suggest new extractants factoring in synthesizability, pH, solubility …





ESCALATE, improved for separation science

Mineva, calculate topological chemical descriptors

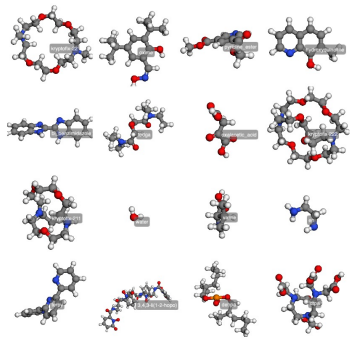
EPO, train DFTB parameters

ADF/Gaussian, DFT calculations

pyiron, complex workflow management package for all-level calculations simultaneously using HPC to enable automatous discovery

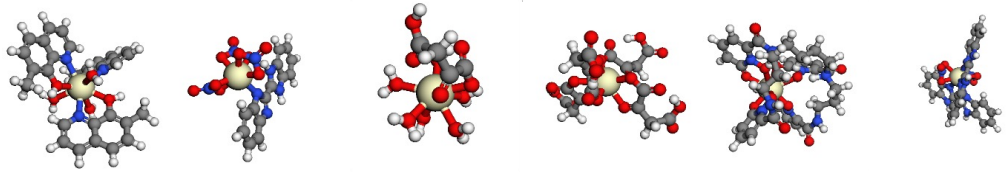
Large-Scale Quantum-based Simulations are needed

Screening of large number of structures

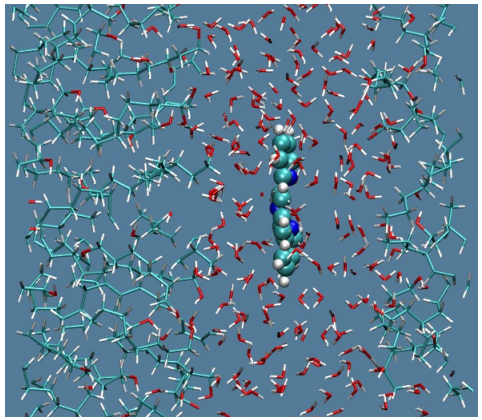


12 extractants, pH depend forms
2 metals, 2 counter ions, 5 conformers

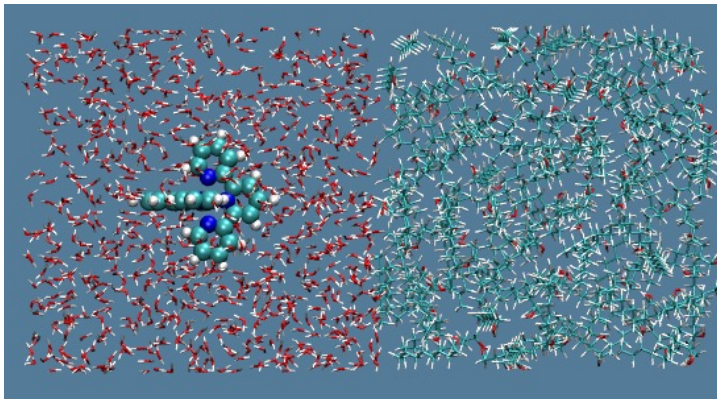
~2200 DFT jobs



Dynamic behavior needs long time scale simulations to cross the interface.



1907 atom
terpy + H_2O + octanol



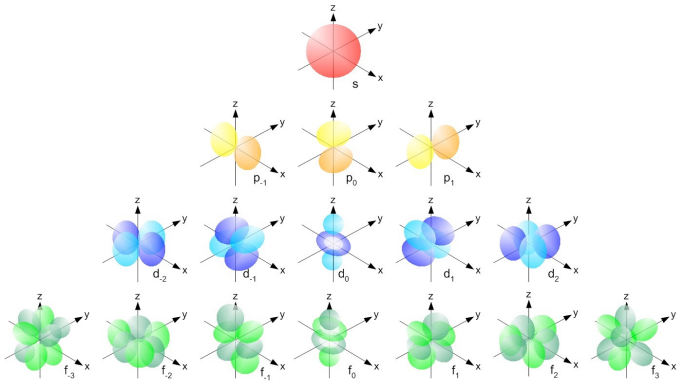
6150 atom ML_2 + H_2O + octanol
Largest SCC-DFTB calculation!

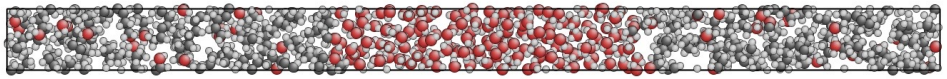
Density Functional Tight Binding (DFTB)

- DFTB is a semi-empirical method derived from DFT

$$E_{DFTB} = \underbrace{\sum_{i}^{occ}\langle\Psi_i|\hat{H}_0|\Psi_i\rangle}_{\text{Band structure energy}} + \underbrace{\frac{1}{2}\sum_{\alpha,\beta}^{N}\gamma_{\alpha\beta}\Delta q_\alpha \Delta q_\beta}_{\text{Charge transfer energy}} + \underbrace{\frac{1}{2}\sum_{\alpha}^{N}\sum_{l}\mathrm{W_l m_l^2}}_{\text{spin energy}} + \underbrace{\frac{1}{2}\sum_{\alpha,\beta}^{N}V_{rep,\alpha,\beta}}_{\text{empirical repulsive pair potential}}$$

- Why DFTB (LATTE)?
  - **Fast:** Roughly ~100X faster than DFT
    - Linear-scaling algorithm available for large systems
    - XLBOMD formalism removes the expensive SCF iterations at each time step
  - **Accurate**
    - DFT level accuracy for forces and energies with good parameterization
    - Self-consistent-charge ensures describing the quantum nature of chemical bonds





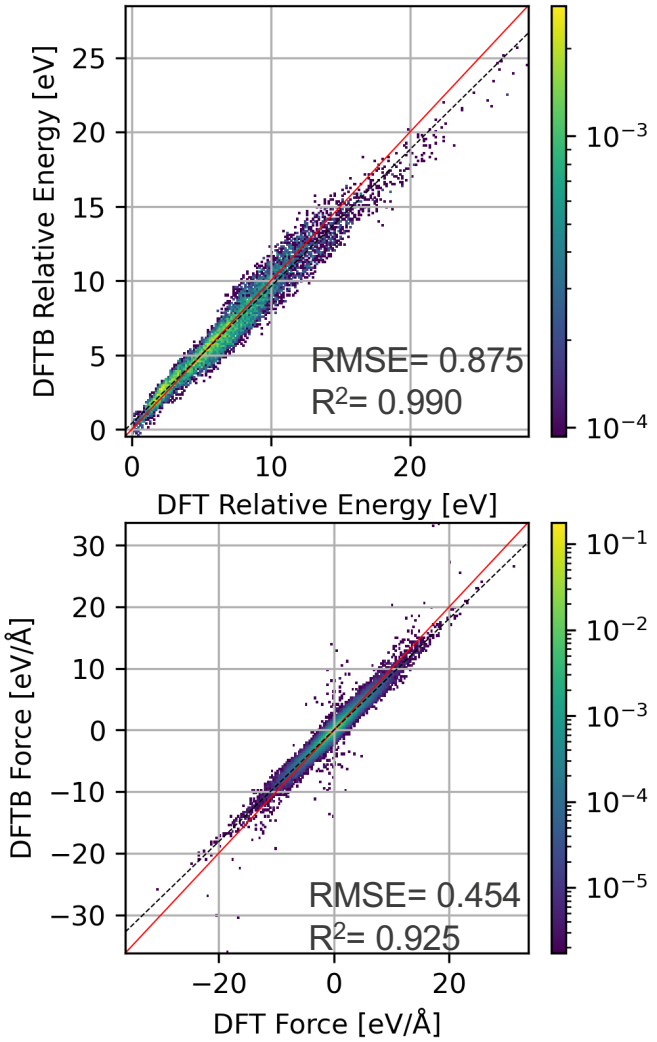
1560 atom H_2O + octanol

Method	Time/time step (s)
Full convergence + diag	1.100
Zero SCF + diag	0.590
Zero SCF + sparse SP2	0.427
Zero SCF + sparse SP2 (GPU)	0.552

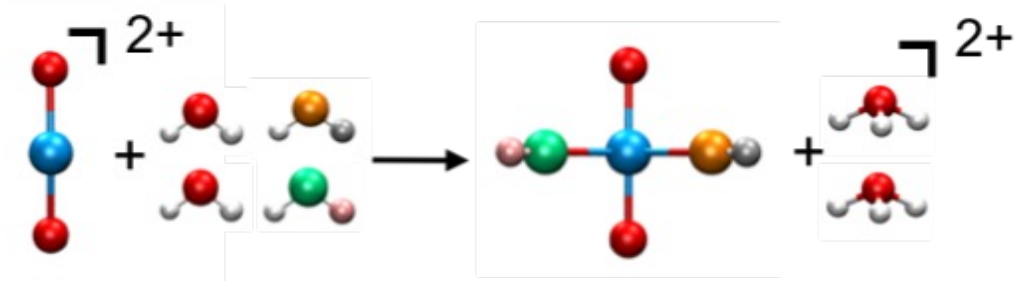
Marc Cawkwell
LANL

DFTB Energies, Forces, and Reactivity

Optimized parameters on n=1-8 clusters



DFTB for Uranium Reactivity



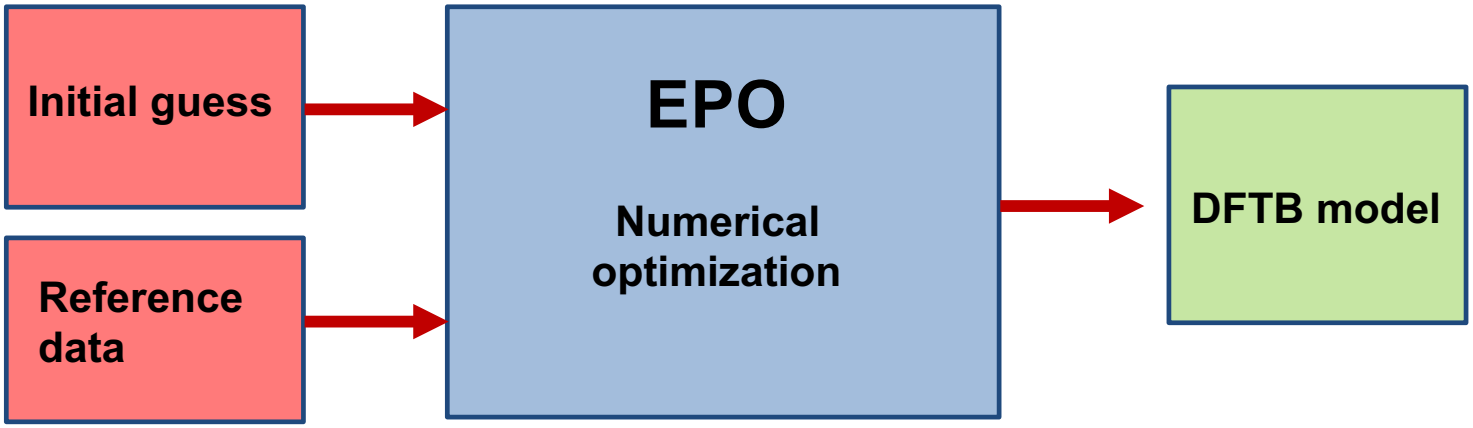
	KS-DFT	DFTB
$UO_2^{2+} + 2H_2O \rightarrow [UO_2(OH)]^+ + H_3O^+$	−7.69	−8.64
$UO_2^{2+} + 4H_2O \rightarrow [UO_2(OH)_2] + 2H_3O^+$	−8.02	−9.44
$[UO_2(OH)]^+ + 2H_2O \rightarrow [UO_2(OH)_2] + H_3O^+$	−0.33	−0.80

Challenges of DFTB parameterization:

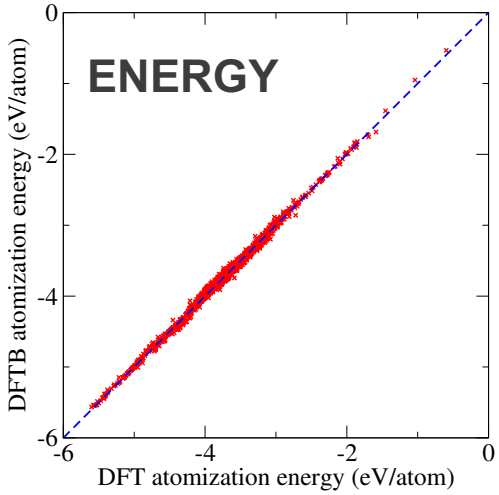
- Large number of parameters
- Limited availability of training data for large chemical space

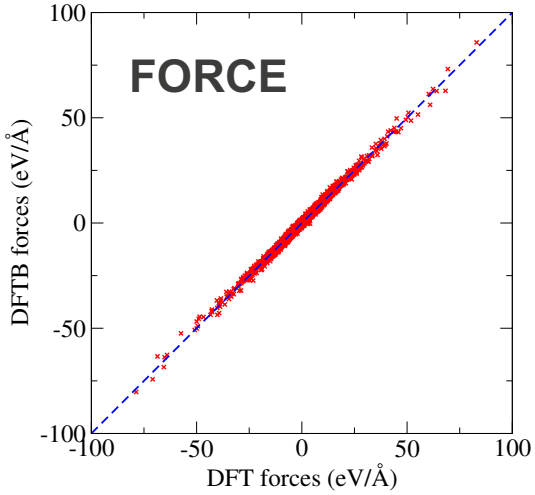
Th-O: Liu, Aguirre, Cawkwell, Batista, Yang, *to be submitted.*
U-O-H: Carlson, Cawkwell, Batista, Yang, JCTC. 2020, **16**, 3073
Am-O-H: Taylor, Burrill, Cawkwell, Lubbers, Batista, Yang, to be submitted

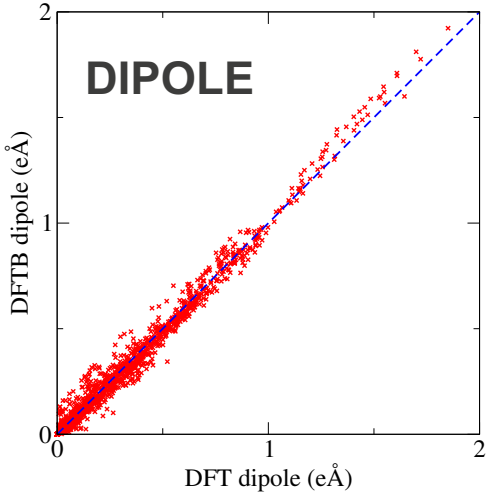
EPO: Parameterization of DFTB for f-Elements



- The 'EPO' code iteratively improves a DFTB parameterization to minimize an objective function that measures the errors in the binding energy and forces vs. DFT.
- Terms needing parameterization are radial dependences of bond integrals and pair potentials, Hubbard U, and on-site energies.

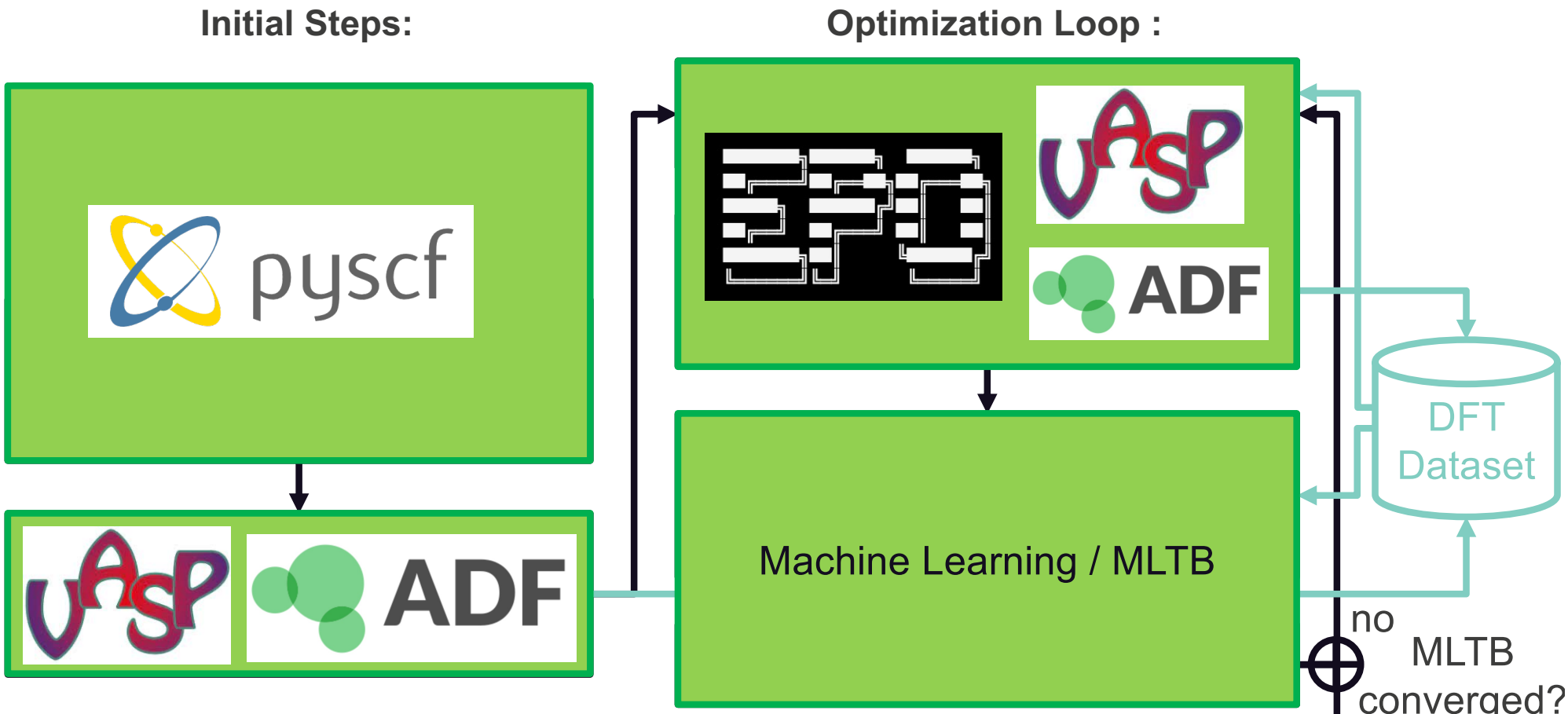






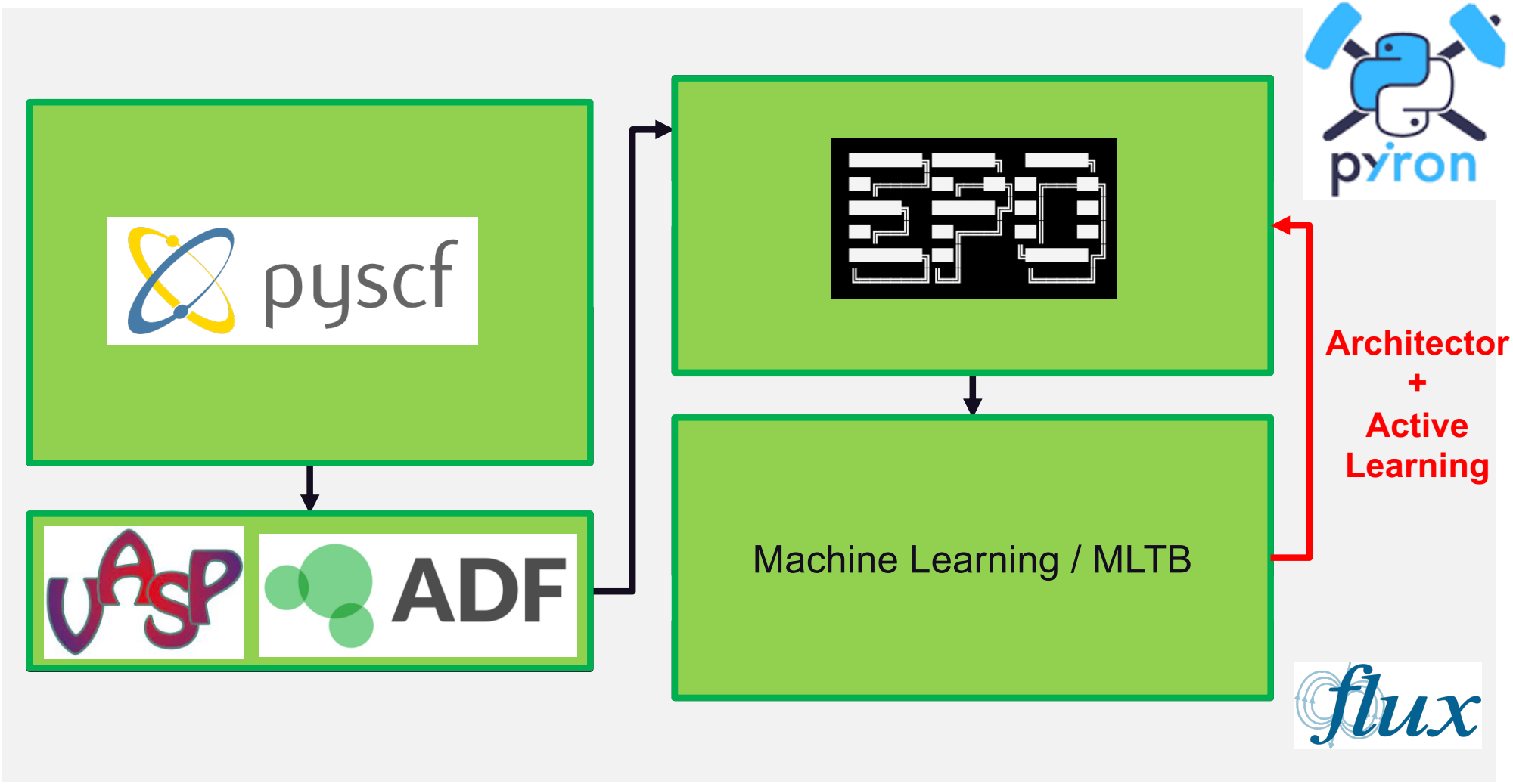
Krishnapriyan, Yang, Niklasson, Cawkwell, *JCTC*, **13**, 6191 (2017)
NF Aguirre, A Morgenstern, MJ Cawkwell, ER Batista, P Yang, Chem. Theory Comp. 2020, 16, 1469

DFTB Training Workflow



- Traditional method requires extensive user knowledge and careful training
- Manual effort required for each black/teal arrow

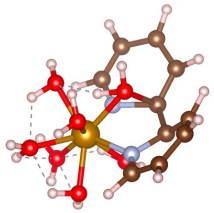
DFTB Training Workflow – Automation Improvements!



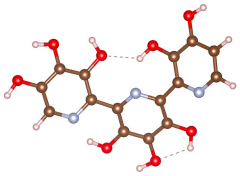
- Extensive Workflow Management Development is underway.

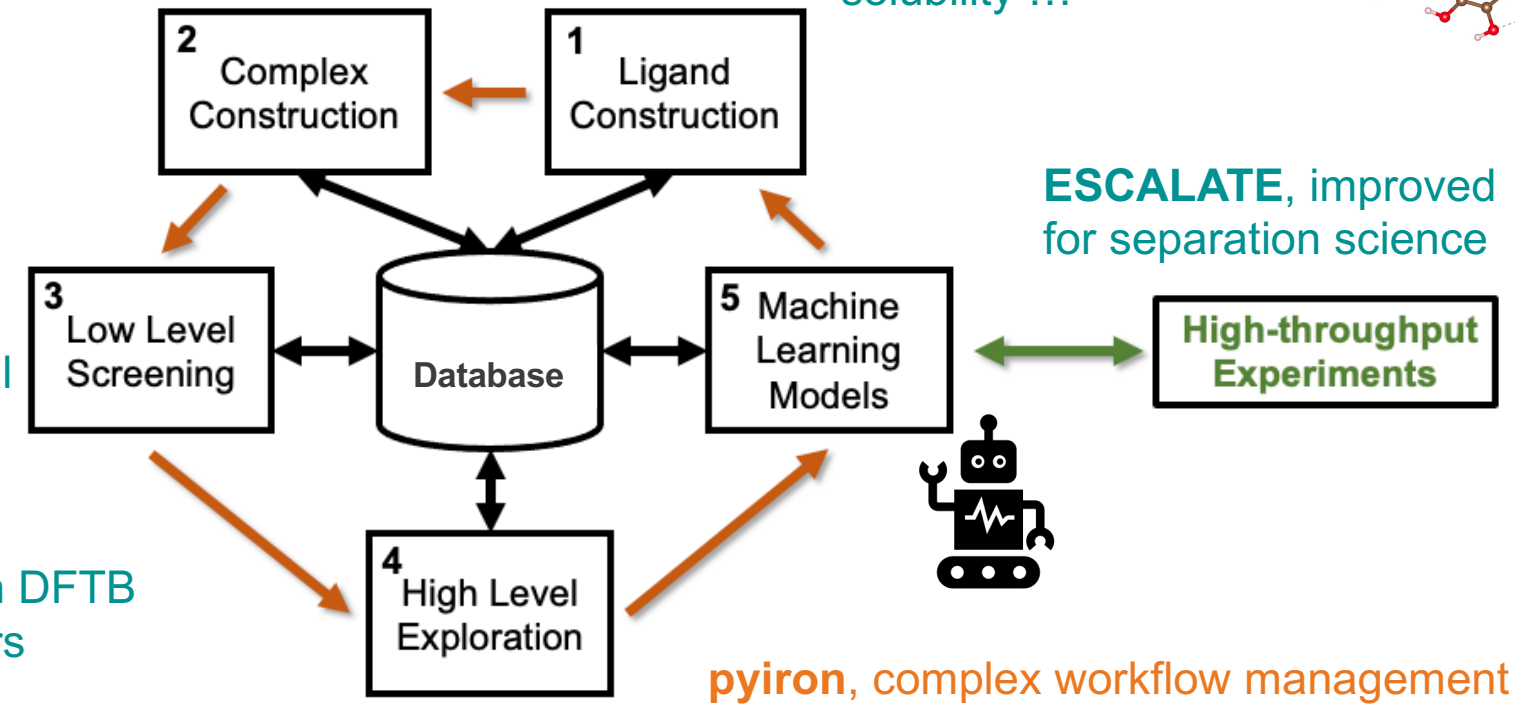
High-throughput Quantum Simulations

Architector, Generate chemically-sensible extractant-actinide complexes



Vulcan, Suggest new extractants factoring in synthesizability, pH, solubility …





ESCALATE, improved for separation science

Mineva, calculate topological chemical descriptors

EPO, train DFTB parameters

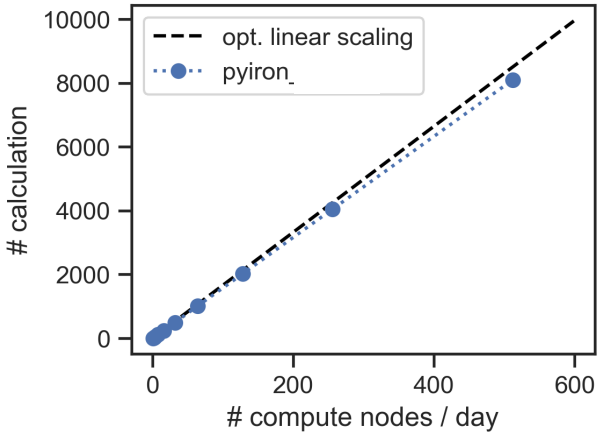
ADF/Gaussian, DFT calculations

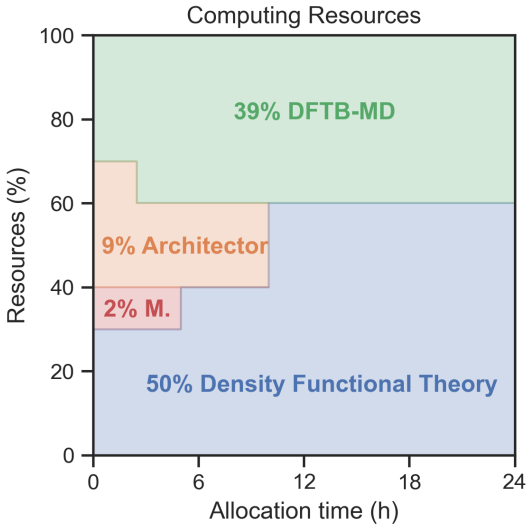
pyiron, complex workflow management package for all-level calculations simultaneously using HPC to enable automatous discovery

Efficient Workflow Management for High-throughput Chemistry Simulations

Enable up-scaling of high-throughput simulations for chemistry

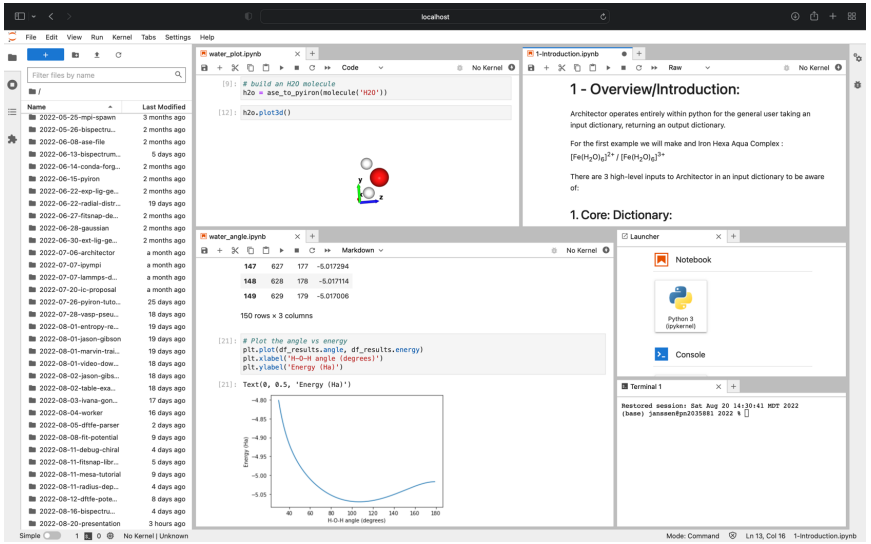
- Developed dynamically-scaling workflow
- Provides simulation protocol provenance
- New interfaces to chemistry codes: ADF, xTB, Gaussian, etc.





Features:

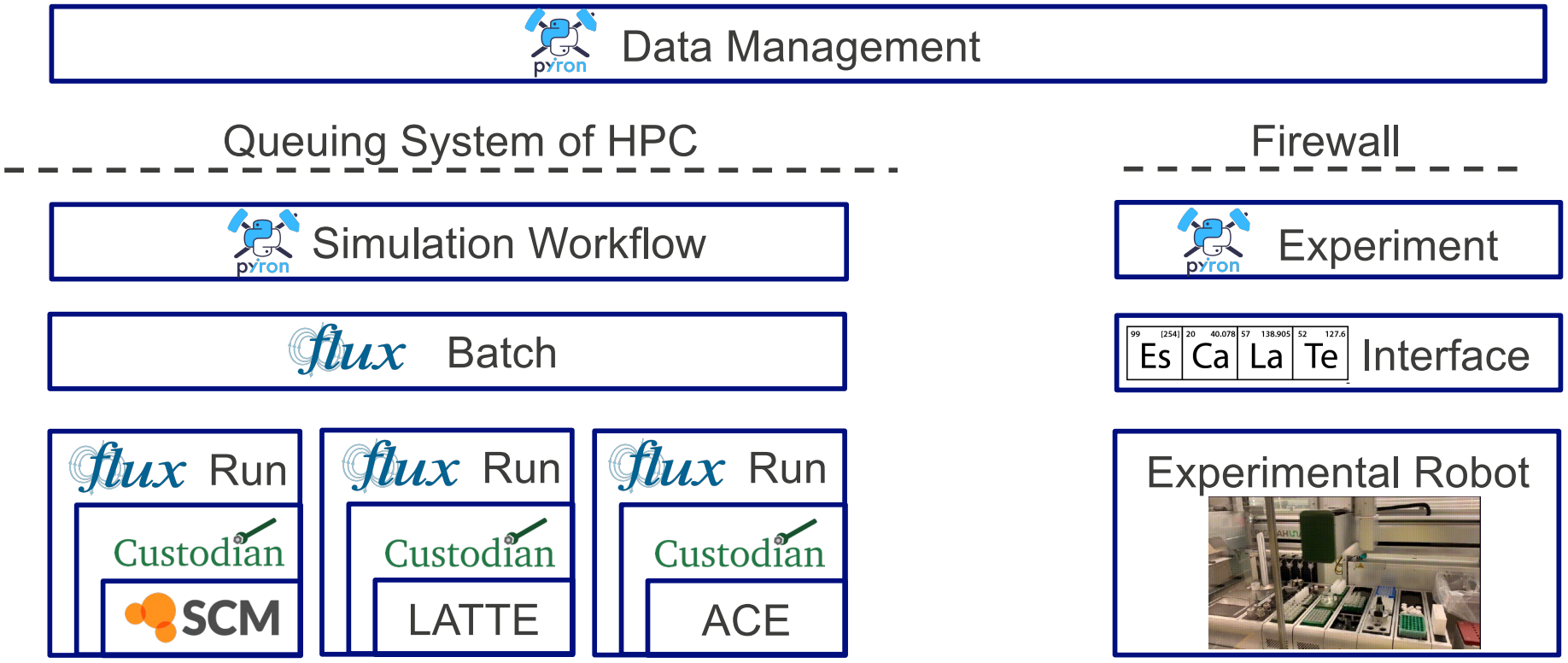
- Highly scalable
- User-friendly interface
- Independent of HPC infrastructure



J. Janssen, et al., Comp. Mat. Sci. 161 (2019) http://pyiron.org

High-throughput Chemistry Simulations at Scale

Construct a complex *hierarchical workflows* with the building blocks you've heard about in this workshop:



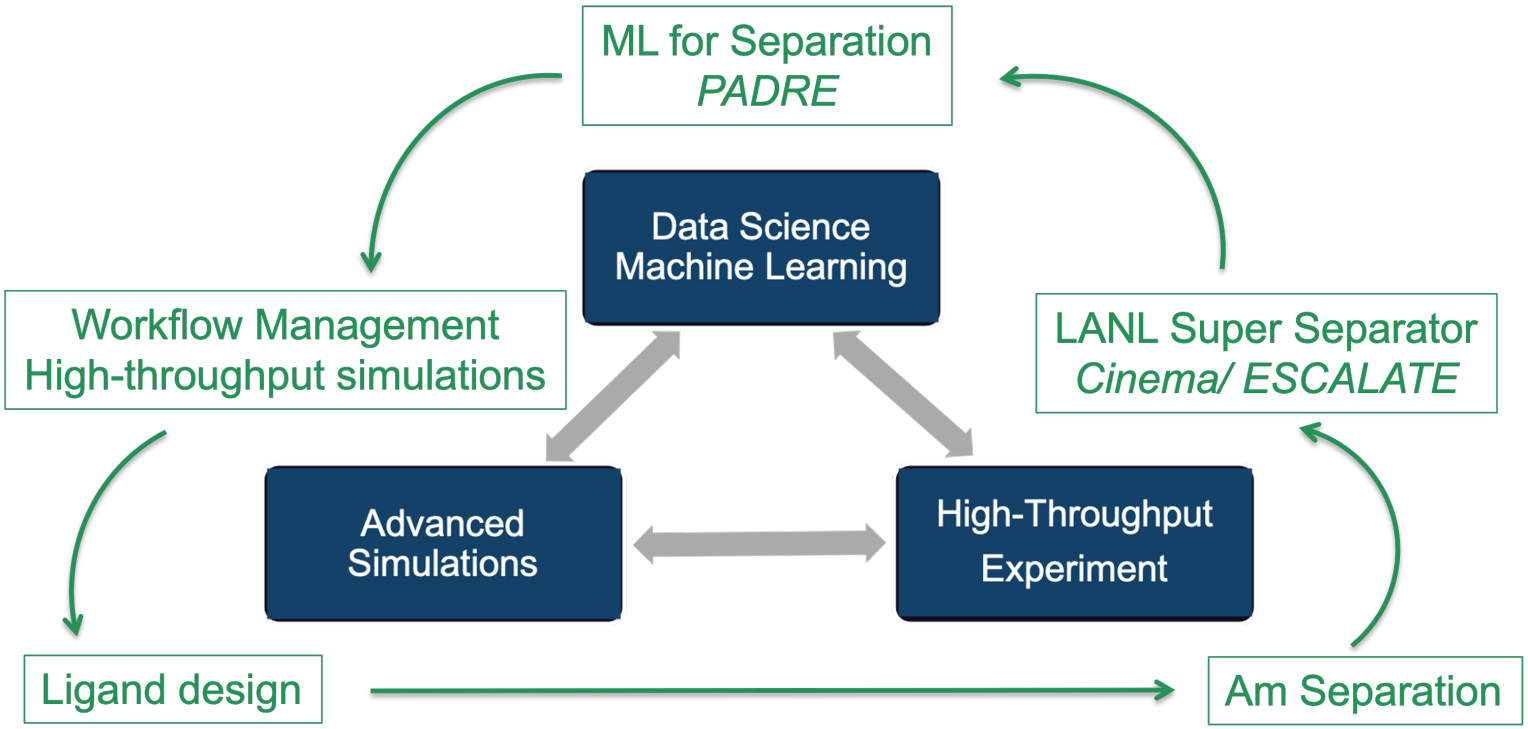
Promising solution coming from this NME IPAM long program!

Michael Taylor
Jan Janssen
Danny Perez

Exascale Future: What is needed?

- Exascale needs:
  - Integration/Centralization of databases across multiple compute resources
  - Strategies for handling calculation/experimental failures.
  - Prioritization strategies for “promising” chemistries (e.g. identify and prioritize chemistries on the fly)
  - Metrics for quality of computational predictions vs. experimental validations.
  - **Hierarchical workflows** need to be interoperable, adaptive, robust such as pyiron+flux

Summary



Robust and interoperative hierarchical workflow management is the key to accelerate discovery of separation science.

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Prof. Graeme Henkelman, University of Texas Austin

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DOE Nuclear Energy Program
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LANL CNLS GRA and Postdoc Fellowships
LANL ISTI GRA and AML Summer School

U.S. DEPARTMENT OF ENERGY | Office of Science

Office of NUCLEAR ENERGY

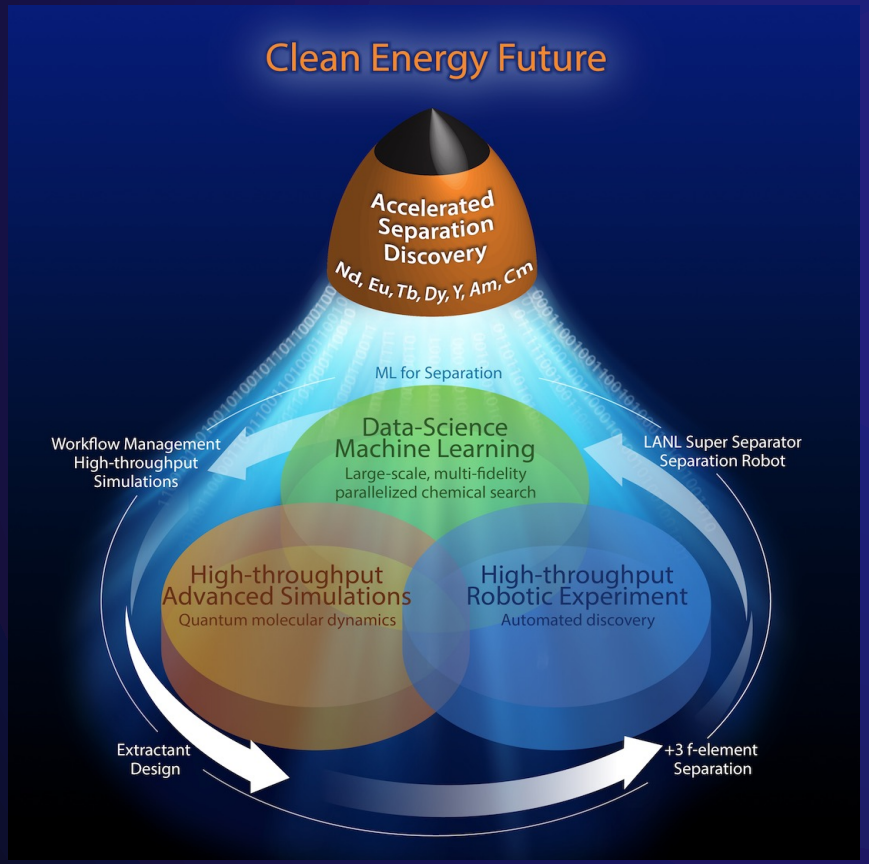
Facilities:

NERSC

LDRD LABORATORY DIRECTED RESEARCH & DEVELOPMENT

Thank you!

pyang@lanl.gov



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