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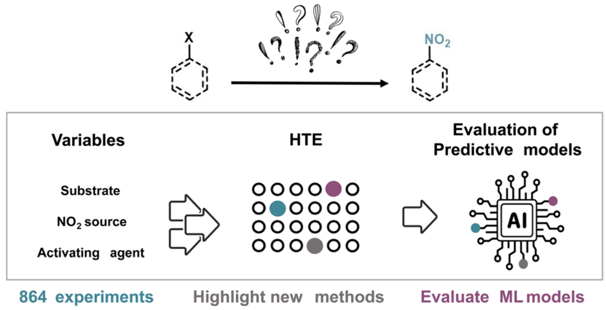
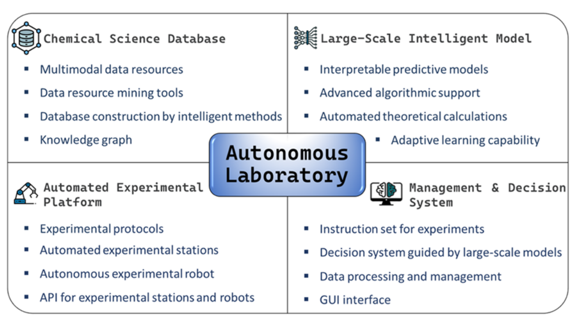
Cover
See Milad Abolhasani *et al.*, pp. 1722–1733. Image reproduced by permission of Milad Abolhasani from *Digital Discovery*, 2025, **4**, 1722.

Inside cover
See Kazunori Nishio, Taro Hitosugi *et al.*, pp. 1734–1742. Image reproduced by permission of Taro Hitosugi from *Digital Discovery*, 2025, **4**, 1734.

COMMUNICATION



PERSPECTIVE



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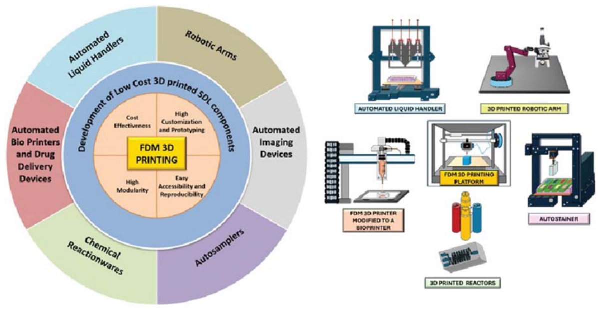
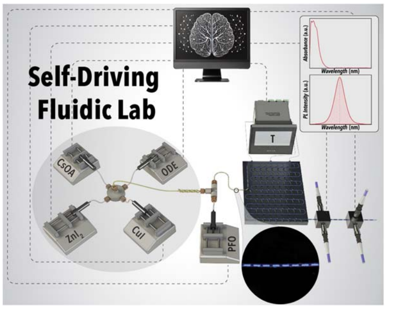
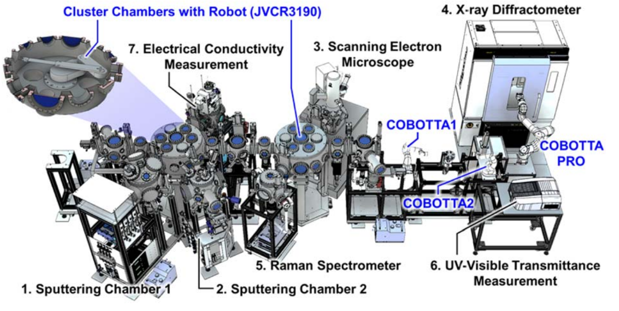
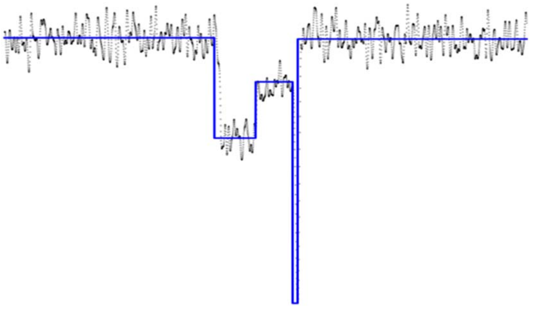
REVIEW



PAPERS







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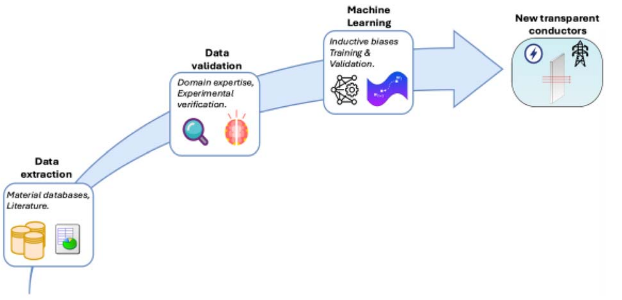
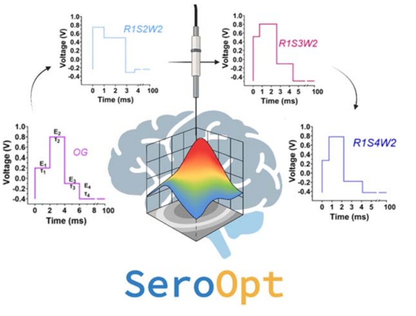
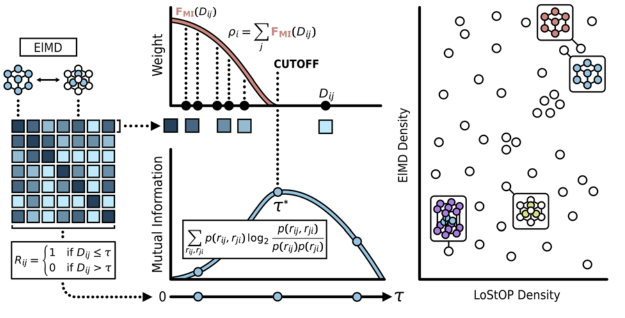
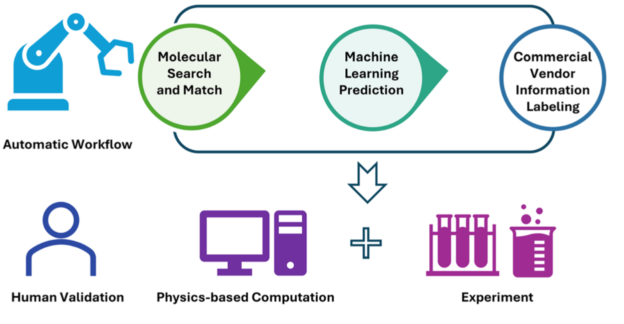
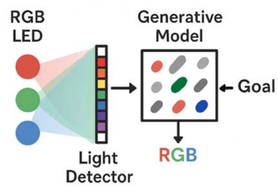

Data extraction
Material databases, Literature.
Data validation
Domain expertise, Experimental verification.
Machine Learning
Inductive biases Training & Validation.
New transparent conductors

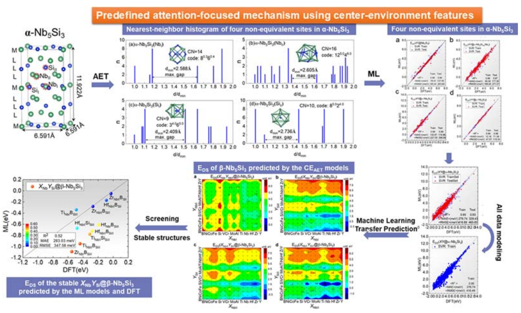

R1S2W2
R1S3W2
OG
R1S4W2
Voltage (V)
Time (ms)
SeroOpt

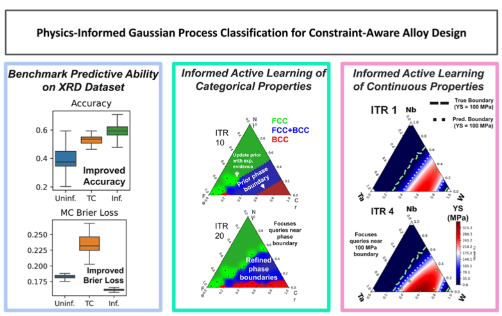

EIMD
Weight
CUTOFF
Mutual Information
EIMD Density
LoStOP Density

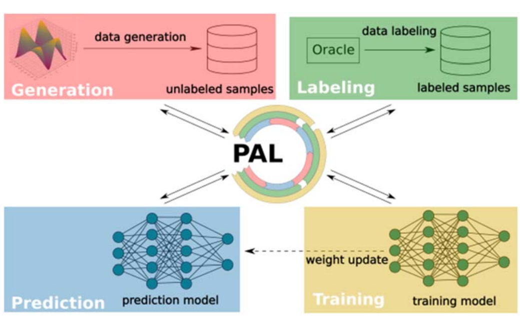

Molecular Search and Match
Machine Learning Prediction
Commercial Vendor Information Labeling
Automatic Workflow
Human Validation
Physics-based Computation
Experiment

PAPERS

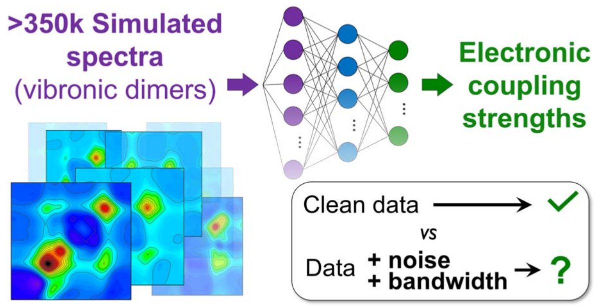

RGB
LED
Generative
Model
Goal
Light
Detector
RGB

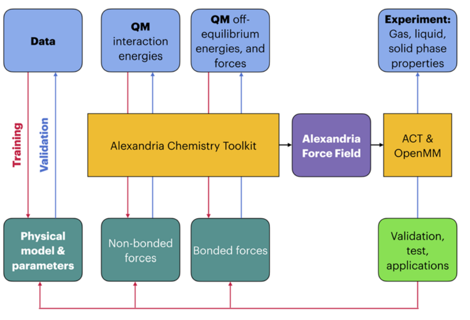

Predefined attention-focused mechanism using center-environment features
AET
ML
Screening
Stable structures
Machine Learning
Transfer Prediction
All data modeling

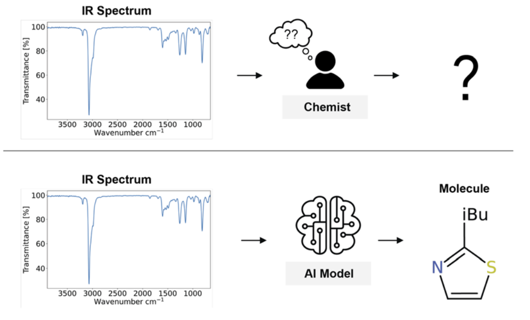

Physics-Informed Gaussian Process Classification for Constraint-Aware Alloy Design
Benchmark Predictive Ability on XRD Dataset
Informed Active Learning of Categorical Properties
Informed Active Learning of Continuous Properties
Accuracy
Improved Accuracy
MC Brier Loss
Improved Brier Loss
ITR 10
ITR 20
FCC
FCC+BCC
BCC
Refined phase boundaries
ITR 1
ITR 4
YS (MPa)

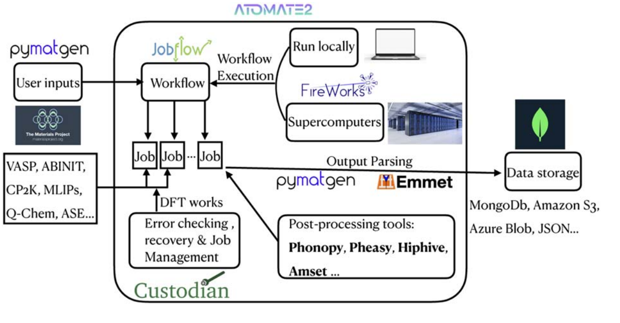

data generation
Generation
unlabeled samples
data labeling
Oracle
Labeling
labeled samples
PAL
Prediction
prediction model
weight update
Training
training model

PAPERS


>350k Simulated spectra
(vibronic dimers)
Electronic coupling strengths
Clean data
vs
Data + noise + bandwidth
?


Data
QM interaction energies
QM off-equilibrium energies, and forces
Experiment: Gas, liquid, solid phase properties
Training
Validation
Alexandria Chemistry Toolkit
Alexandria Force Field
ACT & OpenMM
Physical model & parameters
Non-bonded forces
Bonded forces
Validation, test, applications


IR Spectrum
Transmittance [%]
Wavenumber cm⁻¹
Chemist
?
AI Model
Molecule
iBu
N
S


ATOMATE2
pymatgen
User inputs
Jobflow
Workflow
Workflow Execution
Run locally
FireWorks
Supercomputers
VASP, ABINIT, CP2K, MLIPs, Q-Chem, ASE...
Job
Job
Job
Output Parsing
pymatgen
Emmet
Data storage
MongoDb, Amazon S3, Azure Blob, JSON...
DFT works
Error checking, recovery & Job Management
Post-processing tools: Phonopy, Pheasy, Hiphive, Amset ...
Custodian