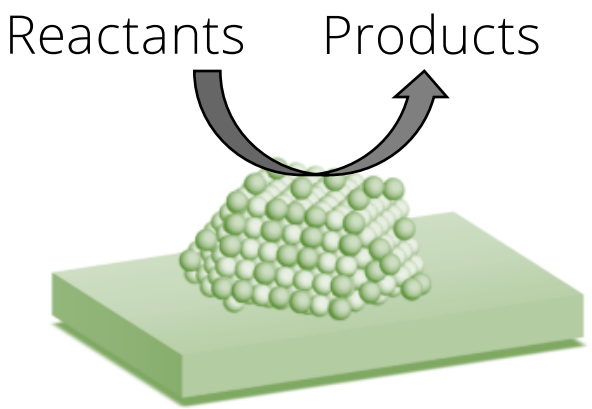
Big-Data Analytics and Machine Learning for Materials Science

Lucas Foppa

The NOMAD Laboratory at the Fritz Haber Institute of the Max Planck Society

Heterogeneous Catalysis: A Materials' Function Governed by an Intricate Interplay of Many Processes



H.-J. Freund *et al*. Angew. Chem. Intl. Ed. 50, 10064 (2011)
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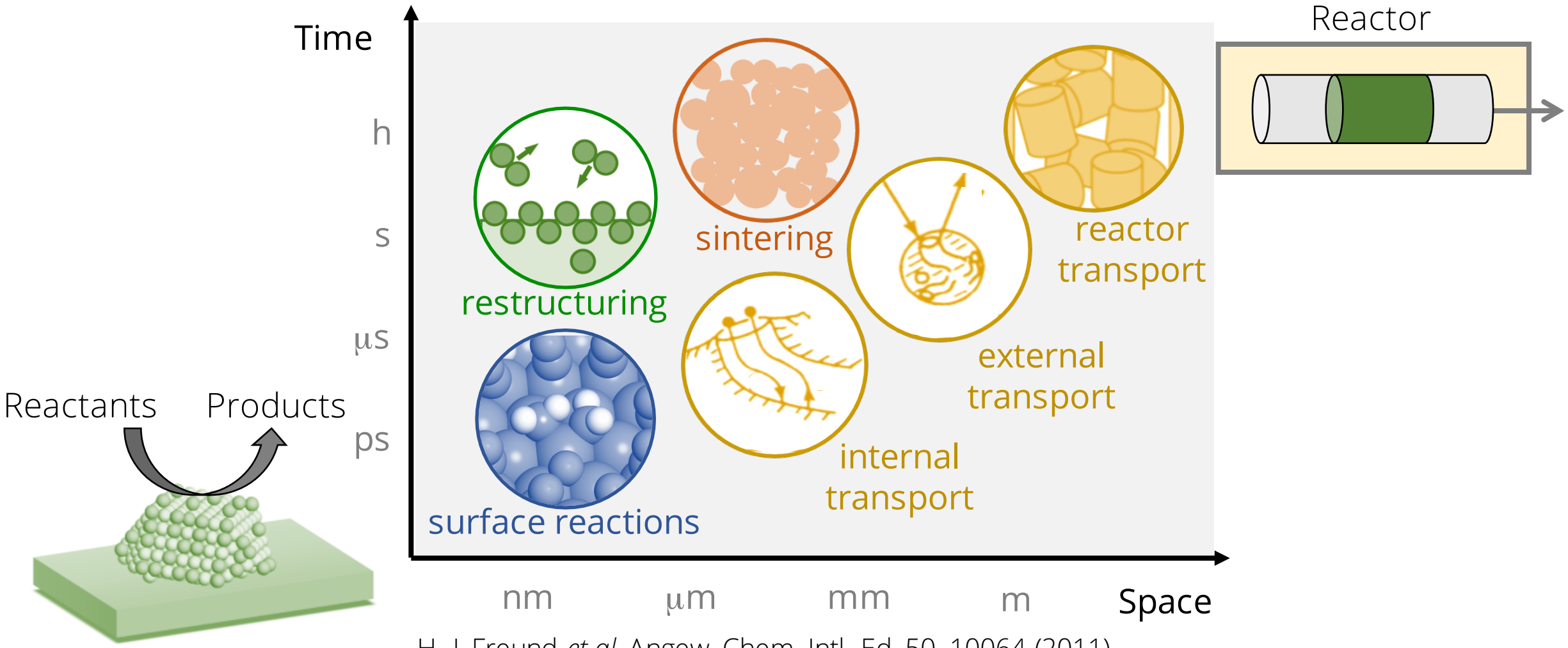

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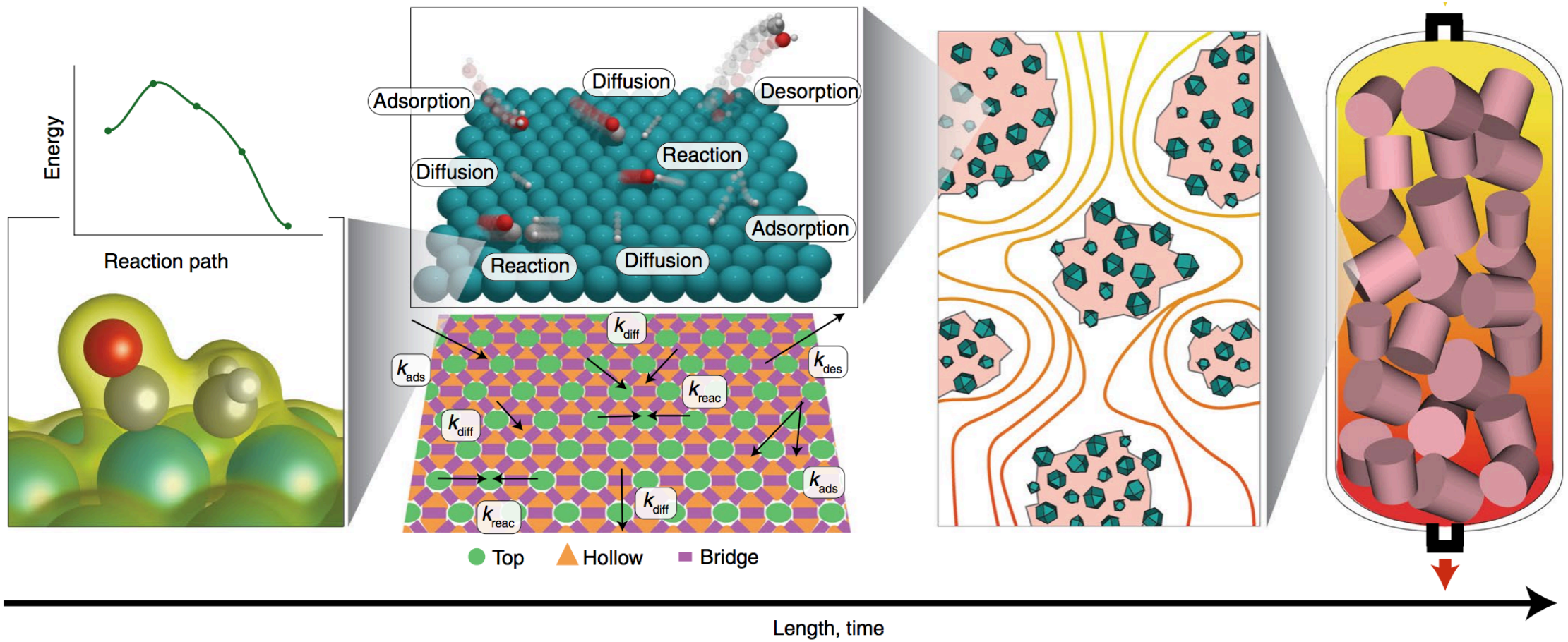
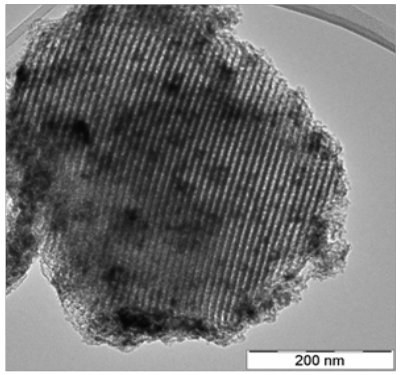
Heterogeneous Catalysis: A Materials' Function Governed by an Intricate Interplay of Many Processes

Explicit Atomistic Models of the Full Catalytic Progression Unfeasible



A. Bruix et al. Nat. Catal. 2, 659 (2019)

Identifying Correlations Describing Materials in Consistent Data with Artificial Intelligence



Systematic Experiments

- Synthesis
- Characterization
- Performance Testing

A. Trunschke *et al.* Top. Catal. 63, 1683 (2020), L. Foppa *et al.* MRS Bull. 46, 1016 (2021), R. Miyazaki *et al.* J. Am. Chem. Soc. 146, 5433 (2024)

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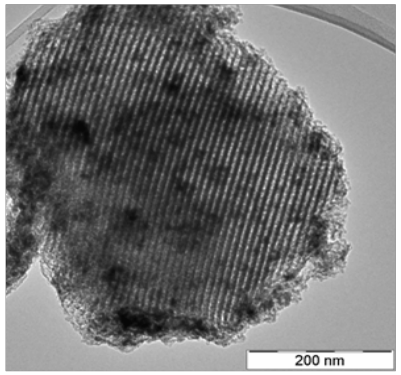

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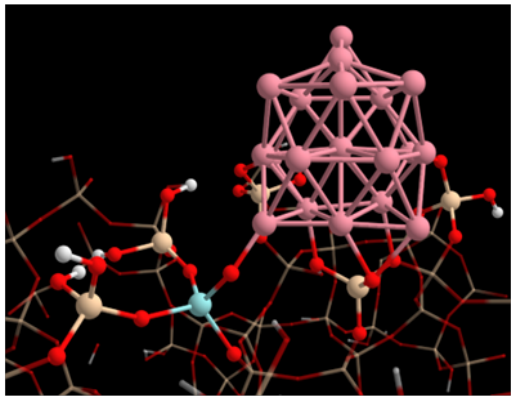
Atomistic Simulations
- Materials Properties
- Environment Effect



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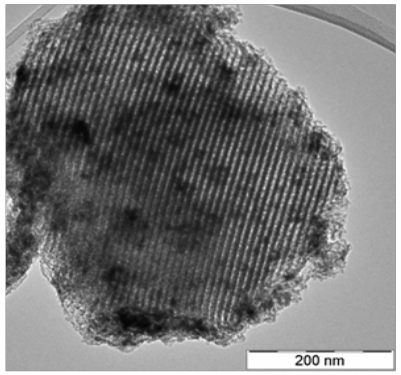

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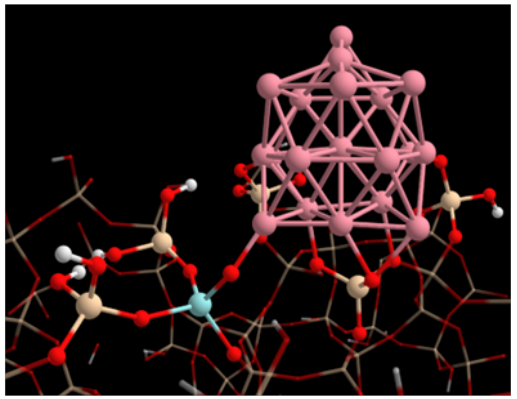

Consistent Dataset
- Target
  - ➢ Measured Performance
- Candidate Descriptive Parameters (Primary Features)
  - ➢ Measured or Calculated
  - ➢ Reflecting Possible Underlying Processes

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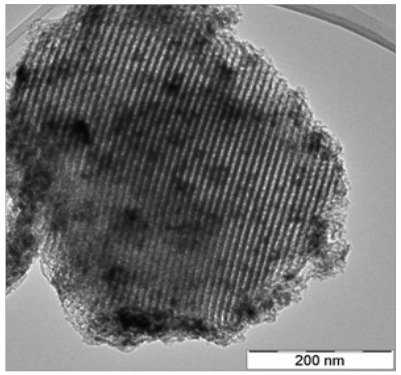

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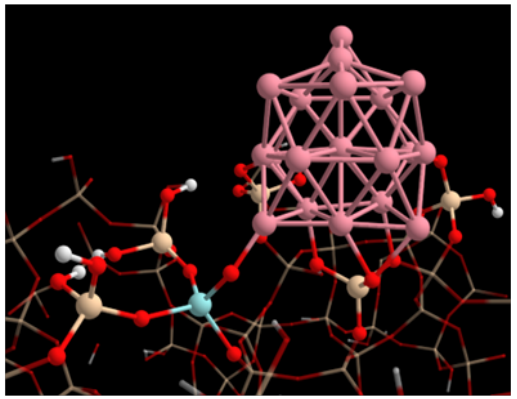

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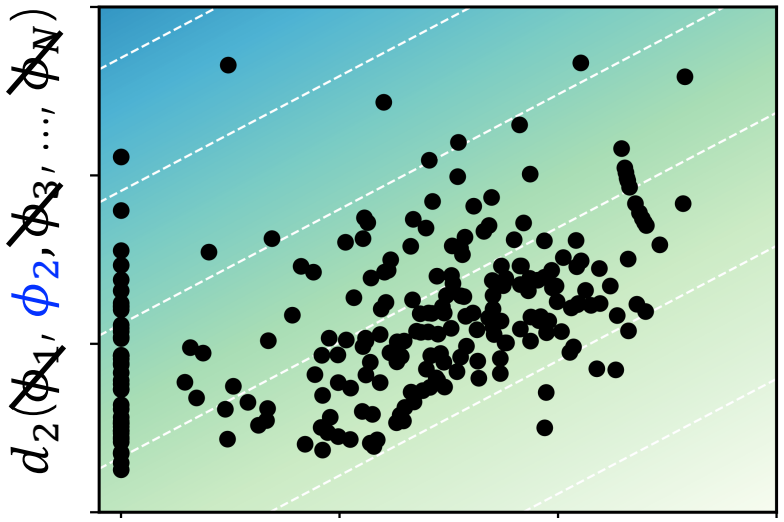
AI

"Materials Genes"

Performance f (Key Parameters)



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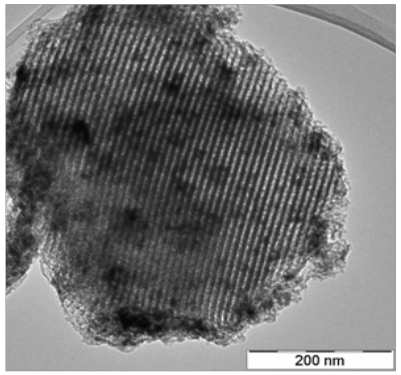

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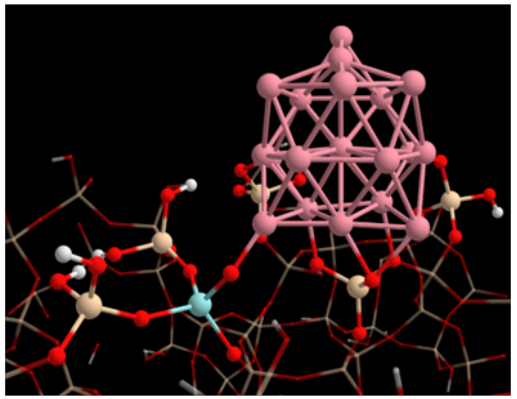

Insights
Predictions

Consistent Dataset
- Target
  - ➢ Measured Performance
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AI

"Materials Genes"

Performance
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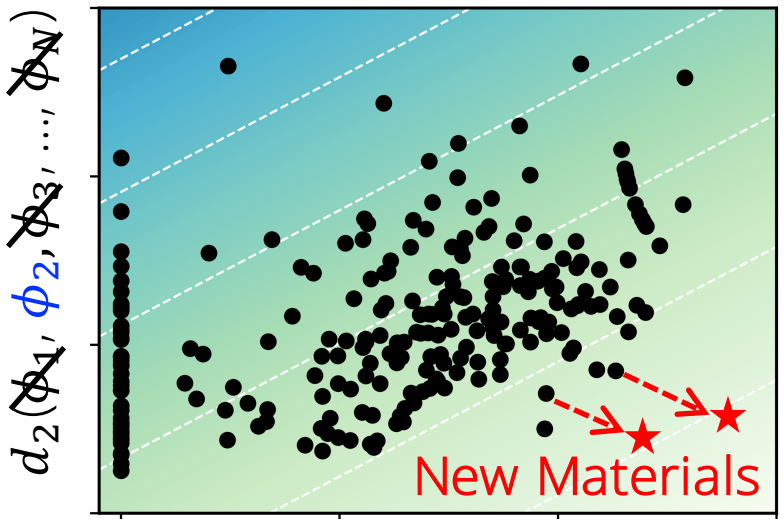

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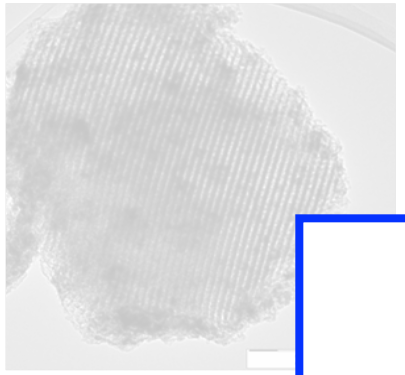

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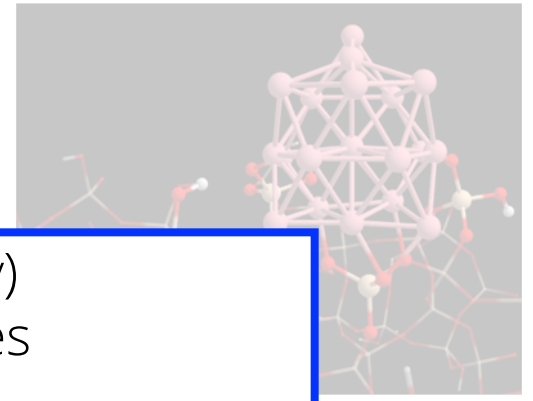
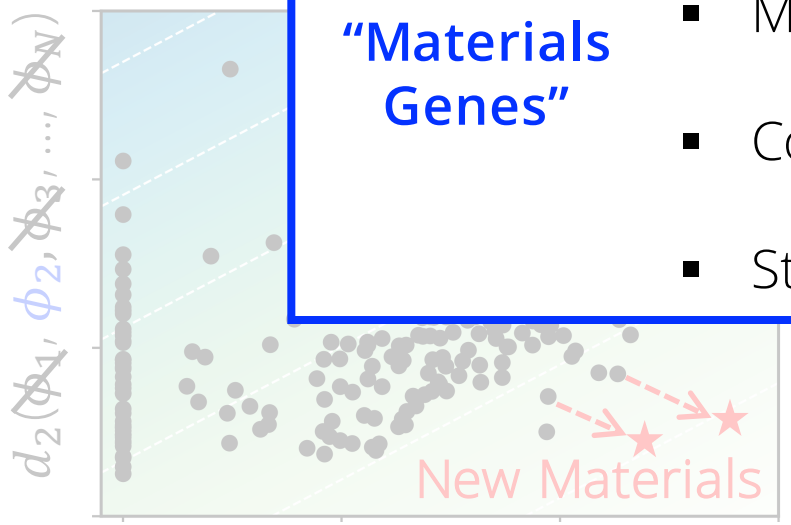


"Materials Genes"

- Capture Complex Patterns But Do Not (Necessarily) Provide Full Understanding of Underlying Processes
- Multiple Parameters
- Correlations (= Rules) Different from Laws
- Statistical Description (Uncertainty, Domain of Applicability)



"Materials Genes"

AI

Primary
- Measured or Calculated
- Reflecting Possible Underlying Processes

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Requirements for AI Methods

- Identification of Key Parameters to Describe Target, From Many Offered Parameters
- Efficient with "Small" Data (e.g., 10^2)

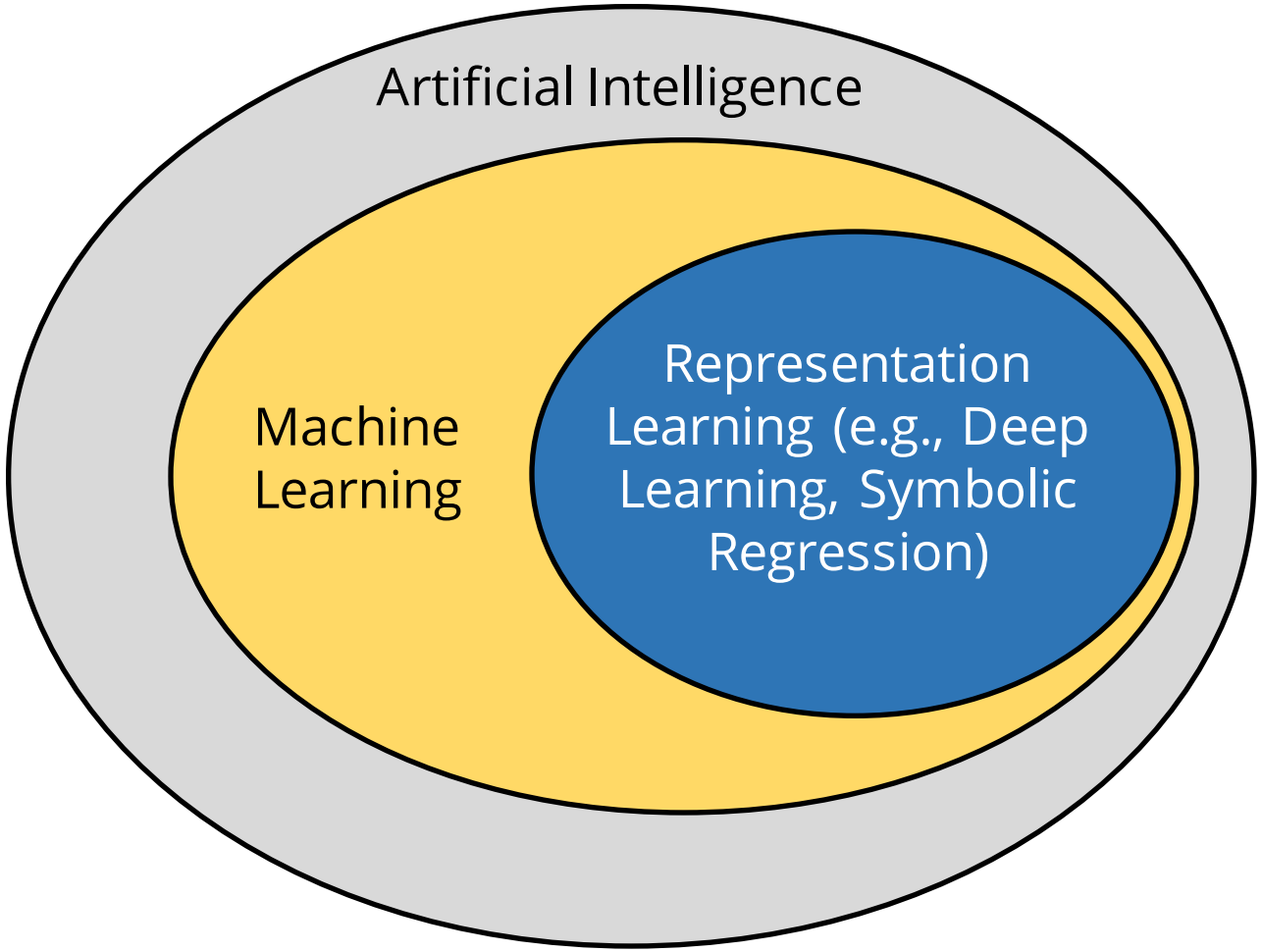

Figure from L. Ghiringhelli

Requirements for AI Methods

- Identification of Key Parameters to Describe Target, From Many Offered Parameters
- Efficient with "Small" Data (e.g., 10^2)
- Methods of Choice:
  - SISSO
  - Subgroup Discovery

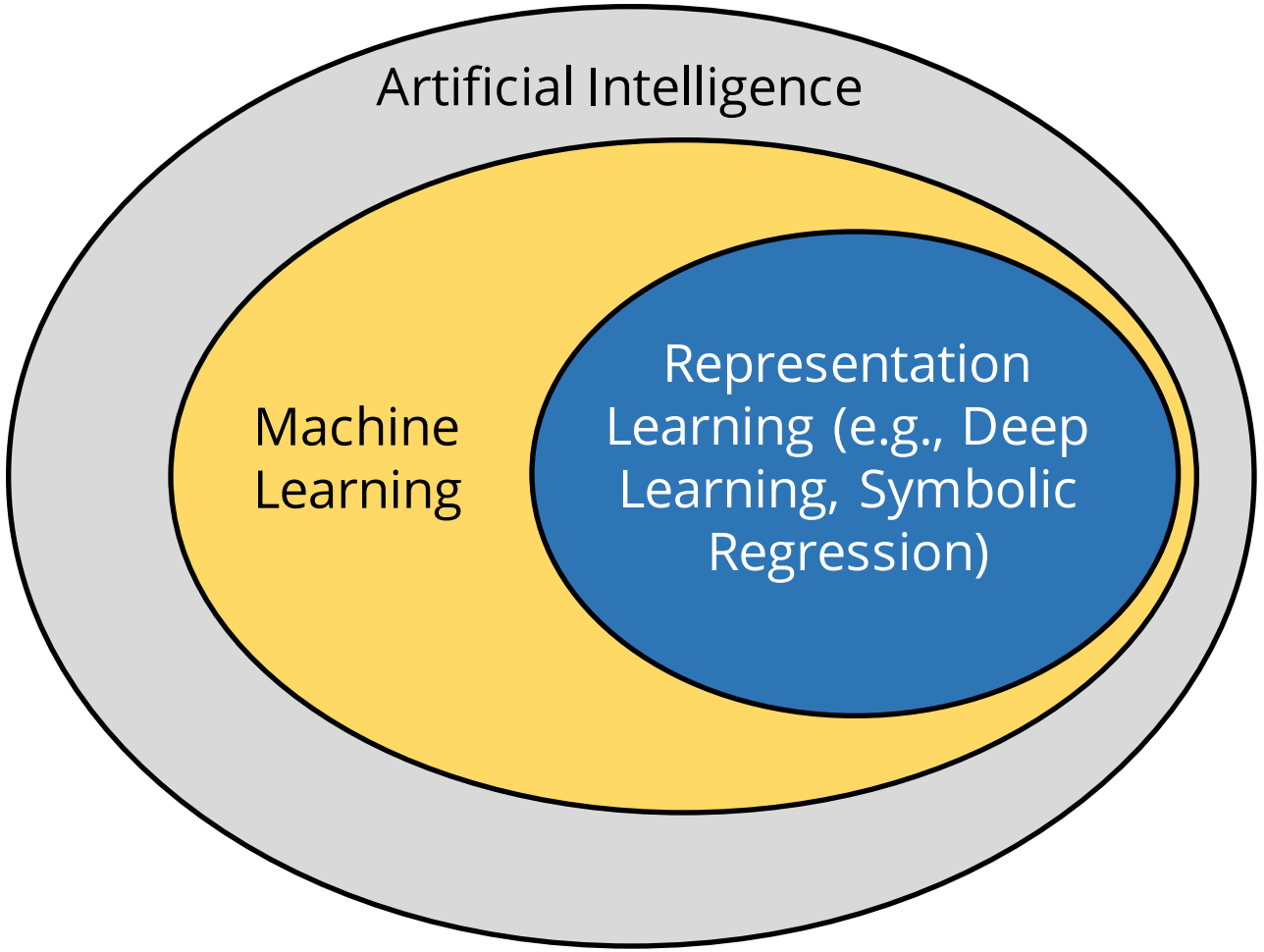

Figure from L. Ghiringhelli

Sure Independence Screening and Sparsifying Operator (SISSO)

1. Choice of Input Parameters (Primary Features, φ_i)

R. Ouyang *et al.* Phys. Rev. Mater. 2, 083802 (2018)
T. A. R. Purcell *et al.* J. Chem. Phys. 159, 114110 (2023)

Sure Independence Screening and Sparsifying Operator (SISSO)

1. Choice of Input Parameters (Primary Features, φ_i)

2. Feature Construction

Primary Feature Space, Φ_0 → Candidate Feature Space, Φ_N

Unary and Binary Mathematical Operators Iteratively Applied

e.g.

$$\varphi_1, \varphi_2 \xrightarrow{q=1} (\varphi_1)^2,\ |\varphi_1 - \varphi_2| \xrightarrow{q=2} \frac{|\varphi_1 - \varphi_2|}{(\varphi_1)^2}$$

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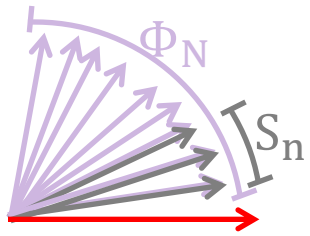
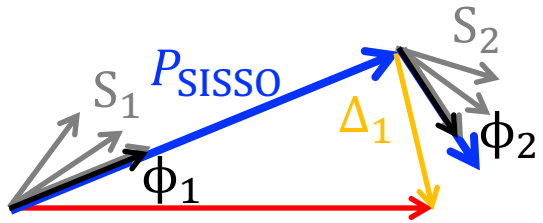
3. Compressed Sensing

Selection SIS → Candidate Feature Subspaces, $\mathbf{S_n}$



P or $\Delta_1, \Delta_2, \Delta_3, \ldots$



P: property
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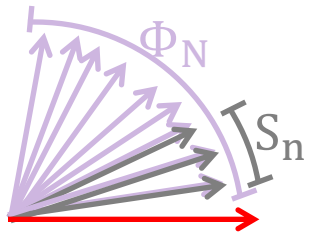
Selection: SIS → Candidate Feature Subspaces, $\mathbf{S_n}$ → Regularization: ℓ_0, SO



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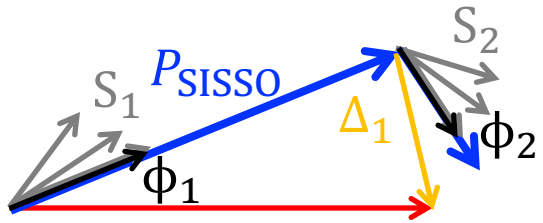

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Descriptor and Model

Fitted Coefficients

$$P^{(\mathrm{SISSO})} = c_0 + \sum_{i=1}^{D} c_i d_i$$

Analytical Expressions

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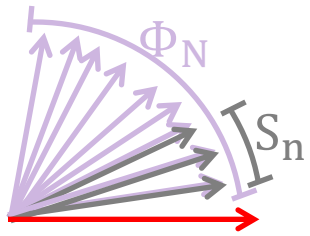

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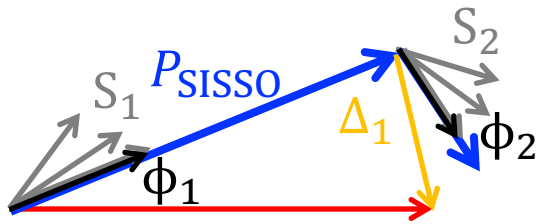

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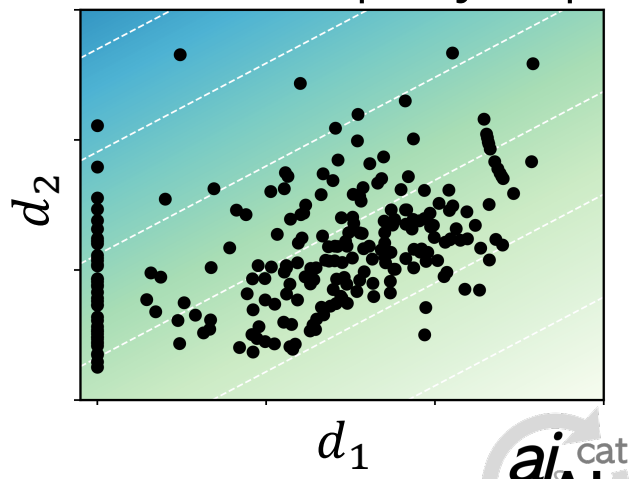
Analytical Expressions

"Materials-Property Maps"



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Immense Number (e.g., billions)

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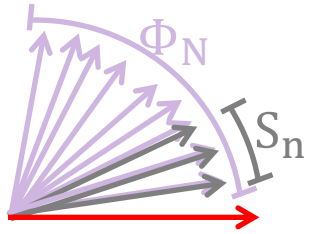

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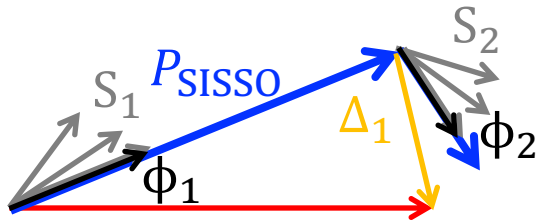

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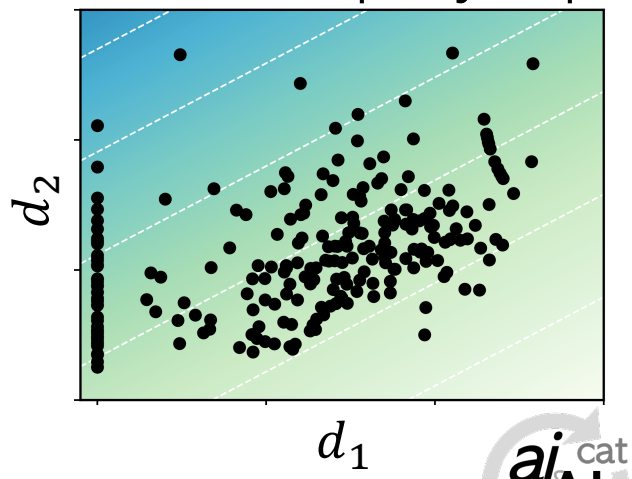

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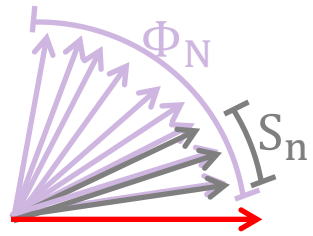
$$\mathcal{L}oss^{\ell_0} = RMSE + \lambda \|\boldsymbol{c}\|_0$$



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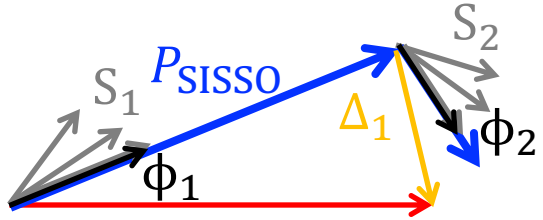

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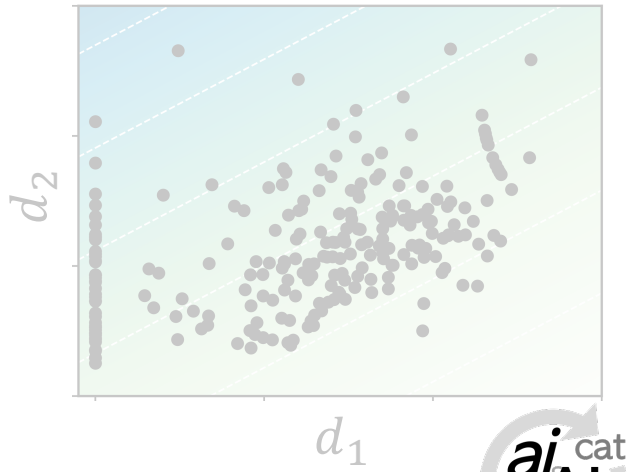

SISSO Handles Larger (Correlated) Feature Spaces than the **LASSO Method** (ℓ_1 Regularization)

$$\mathcal{L}oss^{\ell_1} = RMSE + \lambda \|\boldsymbol{c}\|_1$$

↑ Regularization Strength

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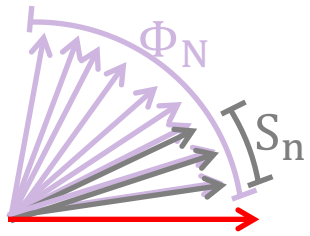

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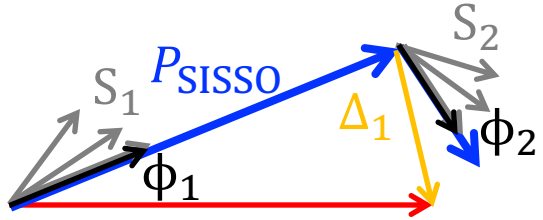

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Analytical Expressions

SISSO Hyperparameters:
D (Dimensionality) and q (Rung)

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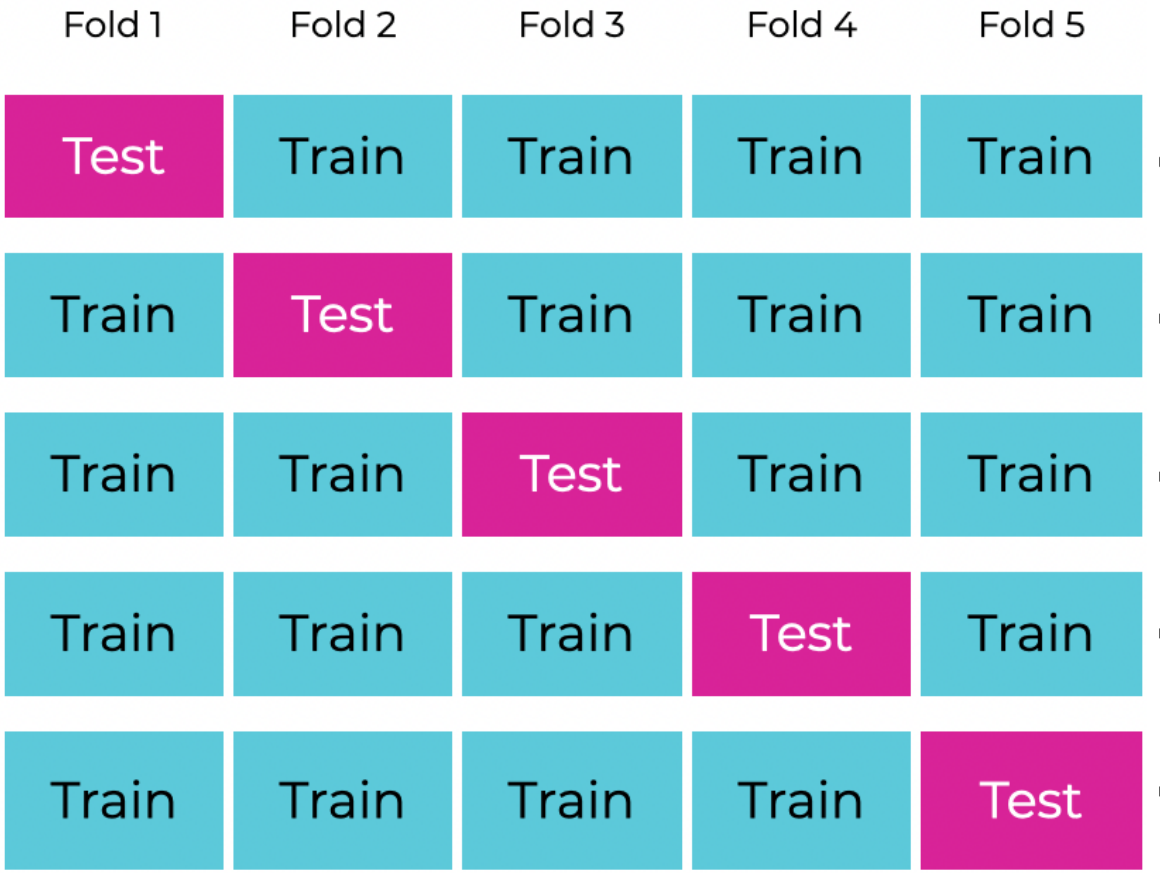
Cross Validation Schemes

- Goals
  - Determine Hyperparameters
  - Estimate Model Performance on Unseen Data
- How?
  - Splitting Dataset into Multiple Folds
  - Training On Some Folds
  - Testing Model Predictions On Other Folds
- Different Schemes Appropriate for Different Problems, e.g., *K*-fold, Nested, and Leave-One-Out

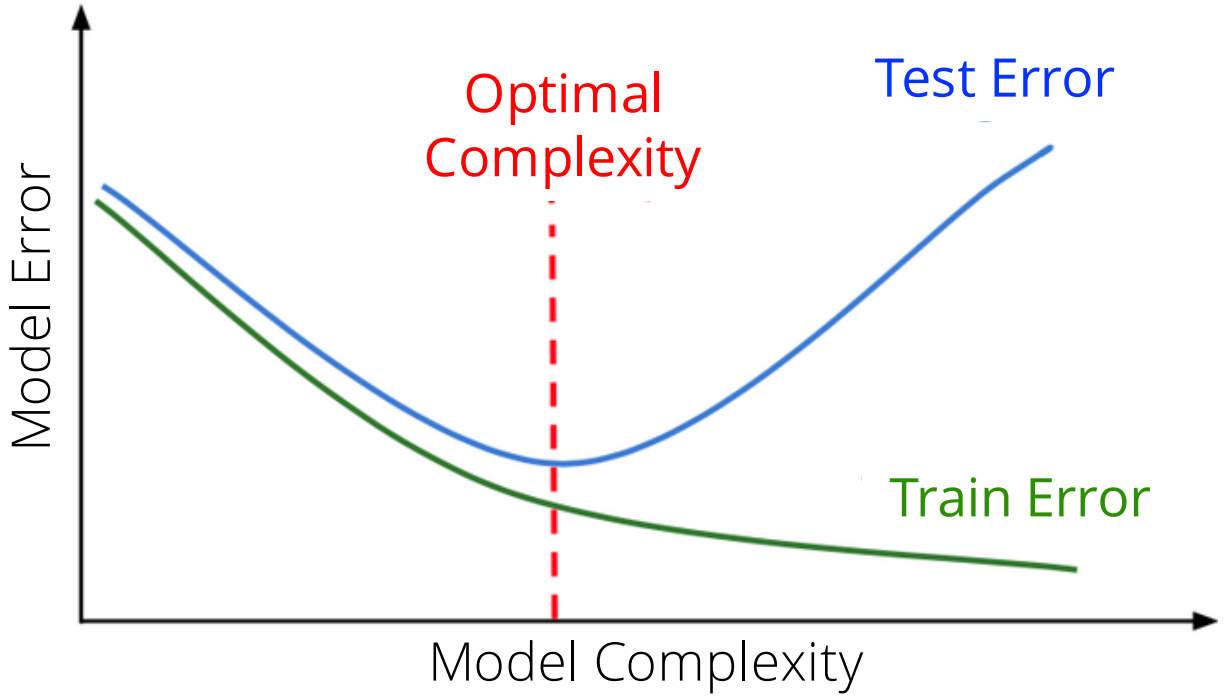
E.g., k-Fold Cross Validation



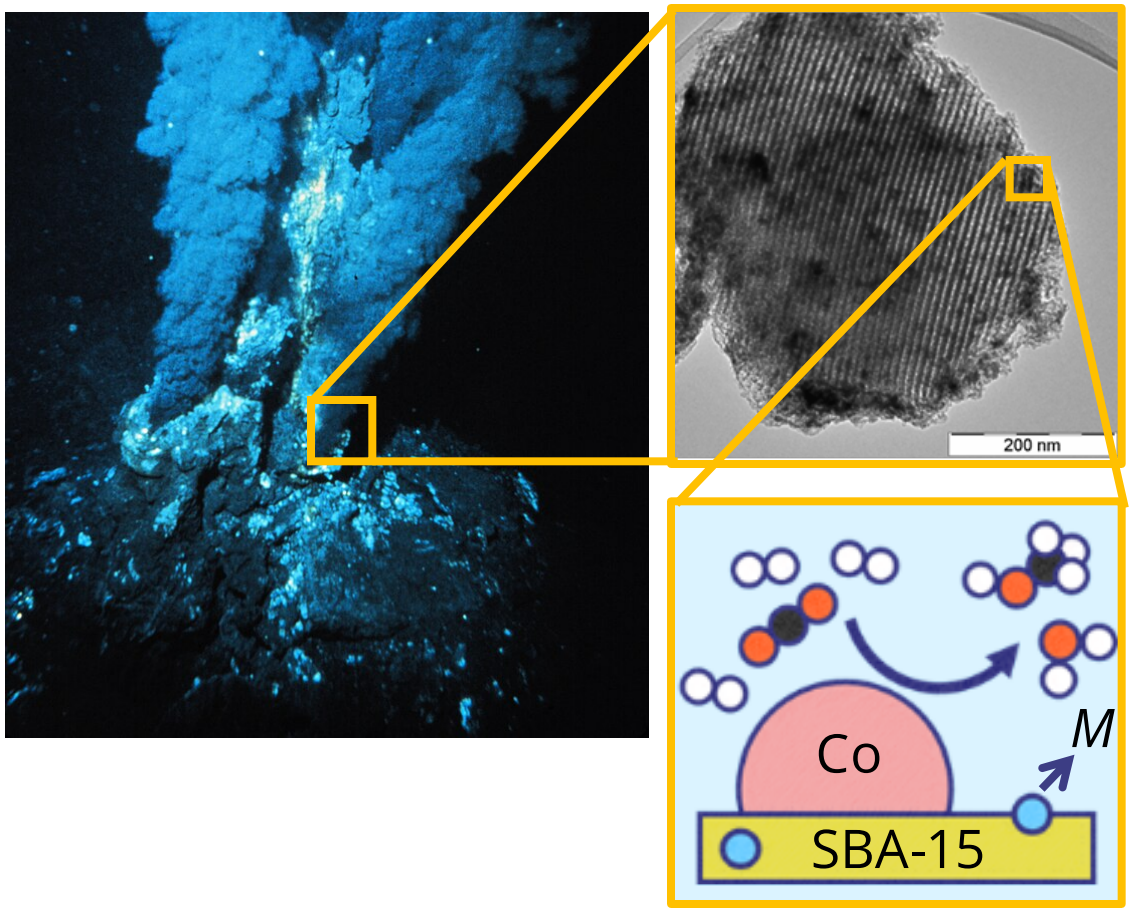
Cross Validation Schemes

- Goals
  - Determine Hyperparameters
  - Estimate Model Performance on Unseen Data
- How?
  - Splitting Dataset into Multiple Folds
  - Training On Some Folds
  - Testing Model Predictions On Other Folds
- Different Schemes Appropriate for Different Problems, e.g., *K*-fold, Nested, and Leave-One-Out

E.g., for Hyperparameters Controlling SISSO Model Complexity D (Dimensionality) and q (Rung)



Application: Describing the Performance of Silica-Supported Cobalt Catalysts (Co/*M*-SiO_2) in CO_2 Hydrogenation



K. Belthle *et al.* J. Am. Chem. Soc. 144, 21232 (2022)

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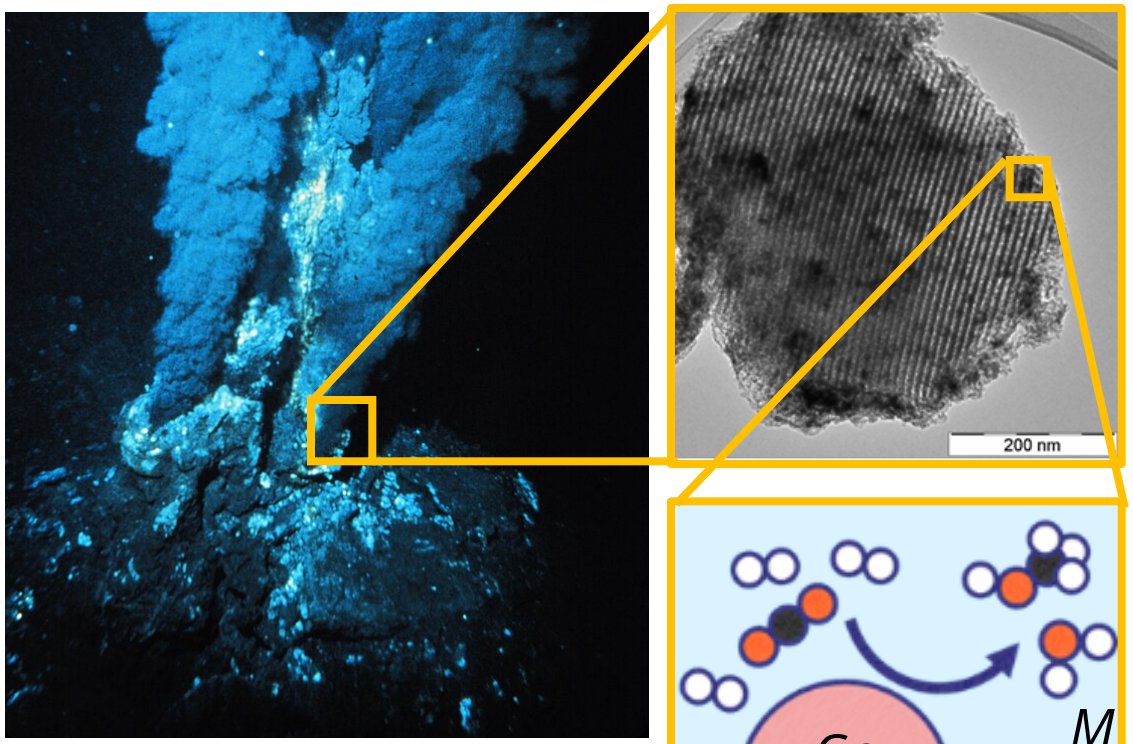

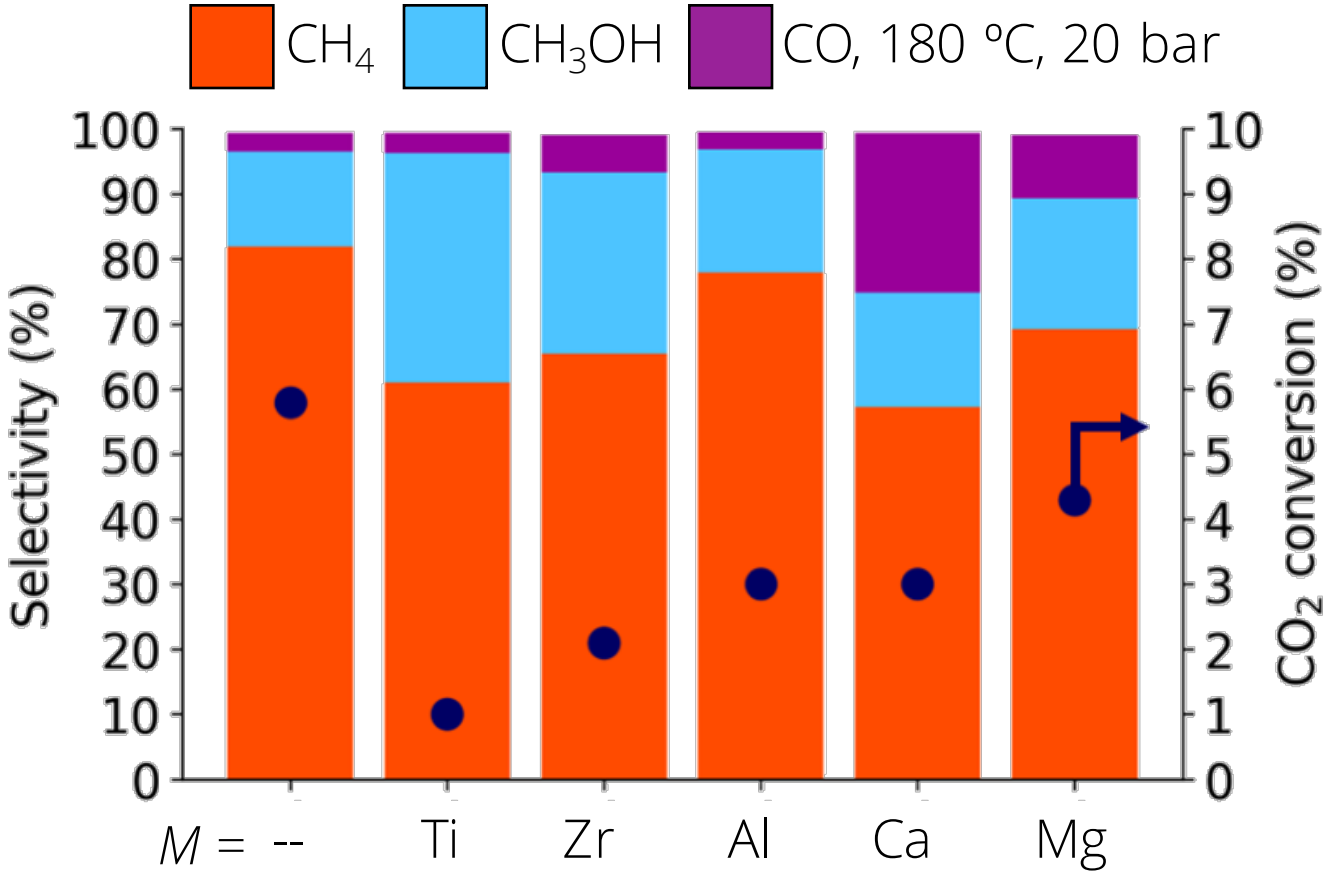

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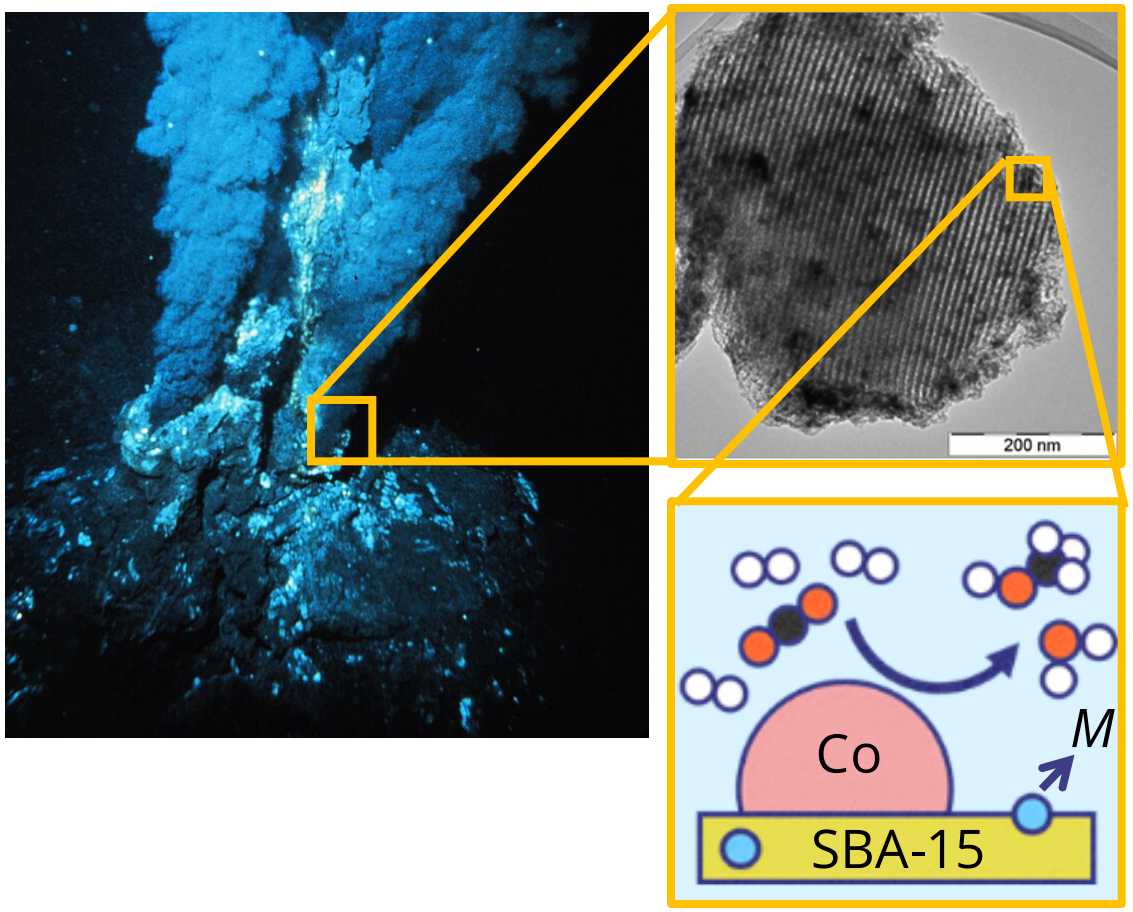

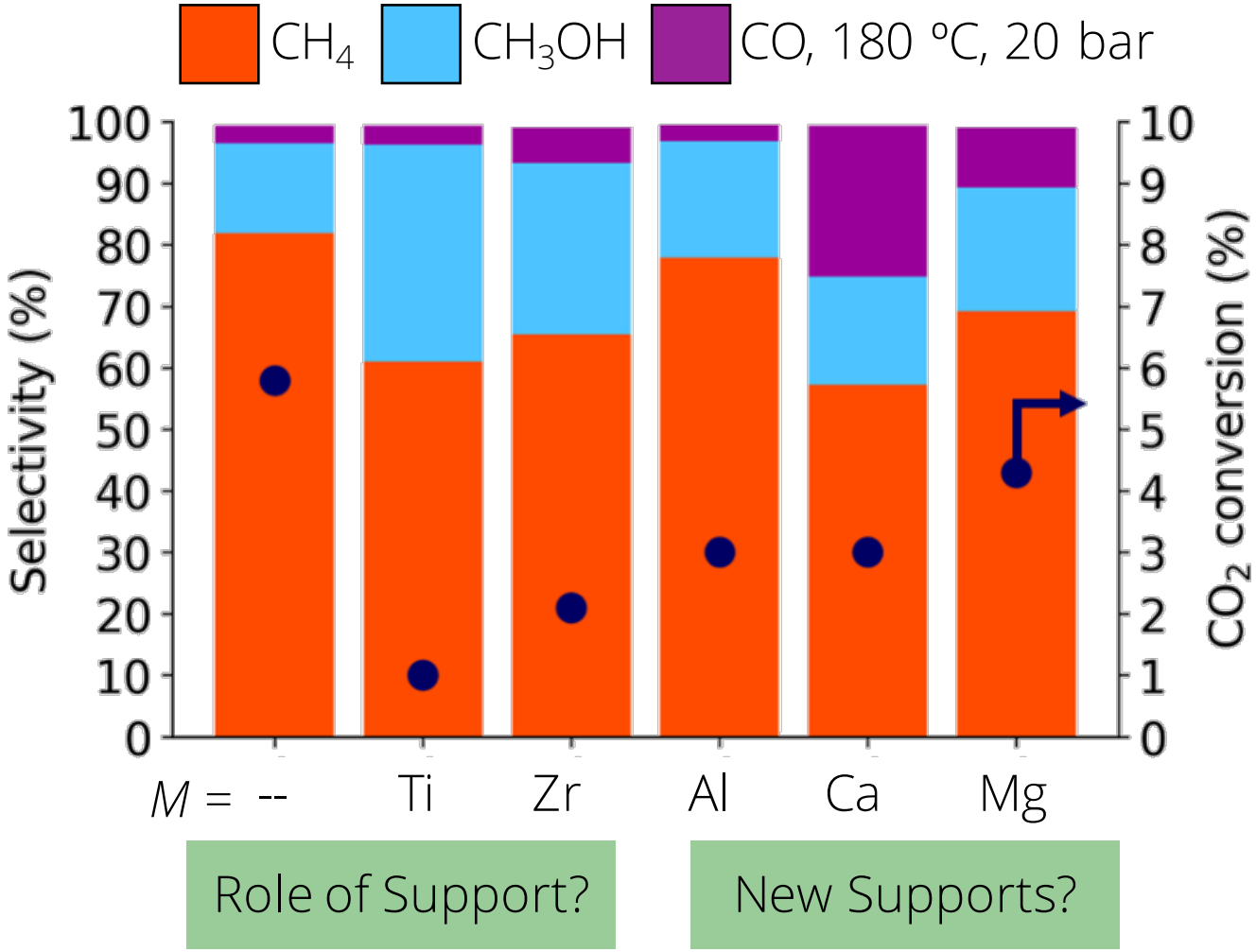

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Application: Describing the Performance of Silica-Supported Cobalt Catalysts (Co/*M*-SiO_2) in CO_2 Hydrogenation

Creating an Experimental-Theoretical Dataset

Measured Performance

Methanol Selectivity

Measured at
4 Reaction Conditions

(6*4=24 data points)

R. Miyazaki *et al.* JACS 146, 5433 (2024)

Application: Describing the Performance of Silica-Supported Cobalt Catalysts (Co/*M*-SiO_2) in CO_2 Hydrogenation

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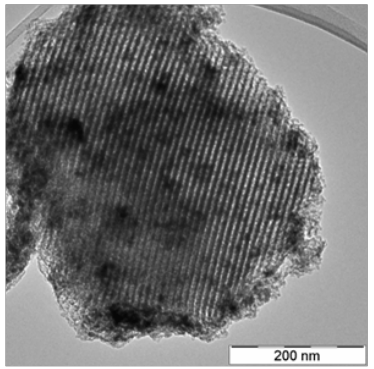

- H_2-TPR
- SEM-EDX
- N_2 adsorption
- CO_2/NH_3-TPD, …

33 Candidate Descriptive Parameters

R. Miyazaki *et al.* JACS 146, 5433 (2024)

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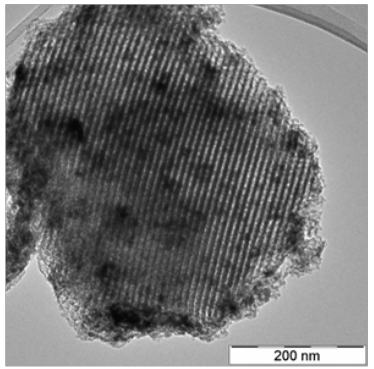

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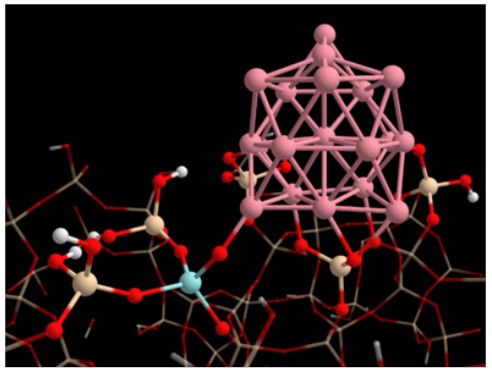
Theoretical



33 Candidate Descriptive Parameters

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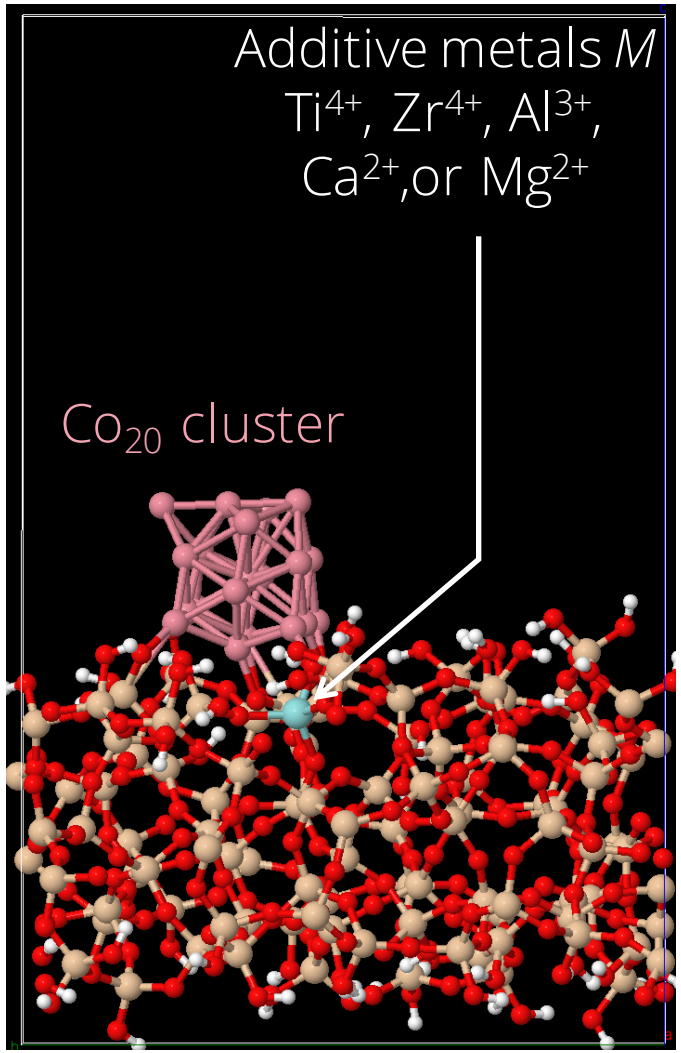
Application: Describing the Performance of Silica-Supported Cobalt Catalysts (Co/*M*-SiO_2) in CO_2 Hydrogenation

Theoretical Candidate Descriptive Parameters

- DFT-RPBE simulations of Co/*M*-SiO_2 interface

FHI-aims
The ab initio materials simulation package

$E_{ads}^{CO_2}$	CO_2 adsorption energy	eV
Δ_{C-O}	C–O bond elongation of adsorbed CO_2	Å
$\Delta_{\angle O-C-O}$	O–C–O angle bending of adsorbed CO_2	degree
q_{CO_2}	Hirshfeld charge of adsorbed CO_2	e
q_M	Hirshfeld charge of the additive metal	e
E_{CH_3O}	CH_3O Formation energy	eV
E_{COOH}	COOH Formation energy	eV
E_{CO+O}	CO + O formation energy	eV
E_{HCOO}	HCOO formation energy	eV
E_{ads}^{O}	O adsorption energy	eV



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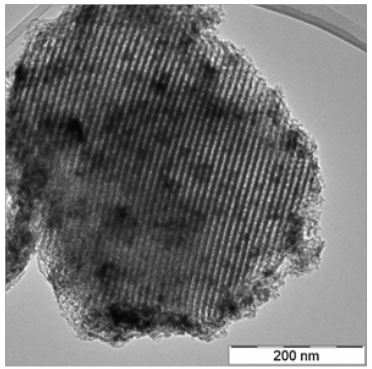

- H_2-TPR
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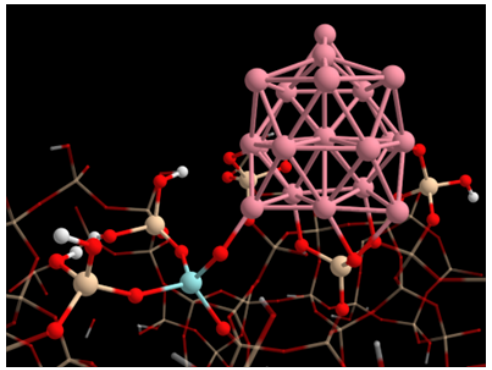
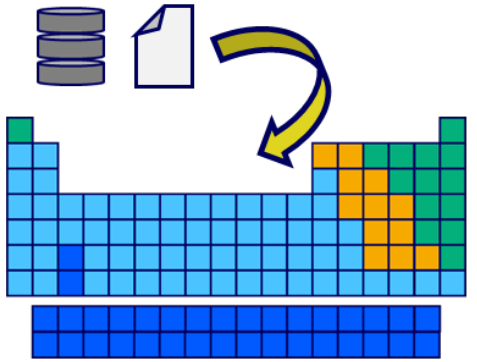


- DFT-RPBE Simulations

Elemental



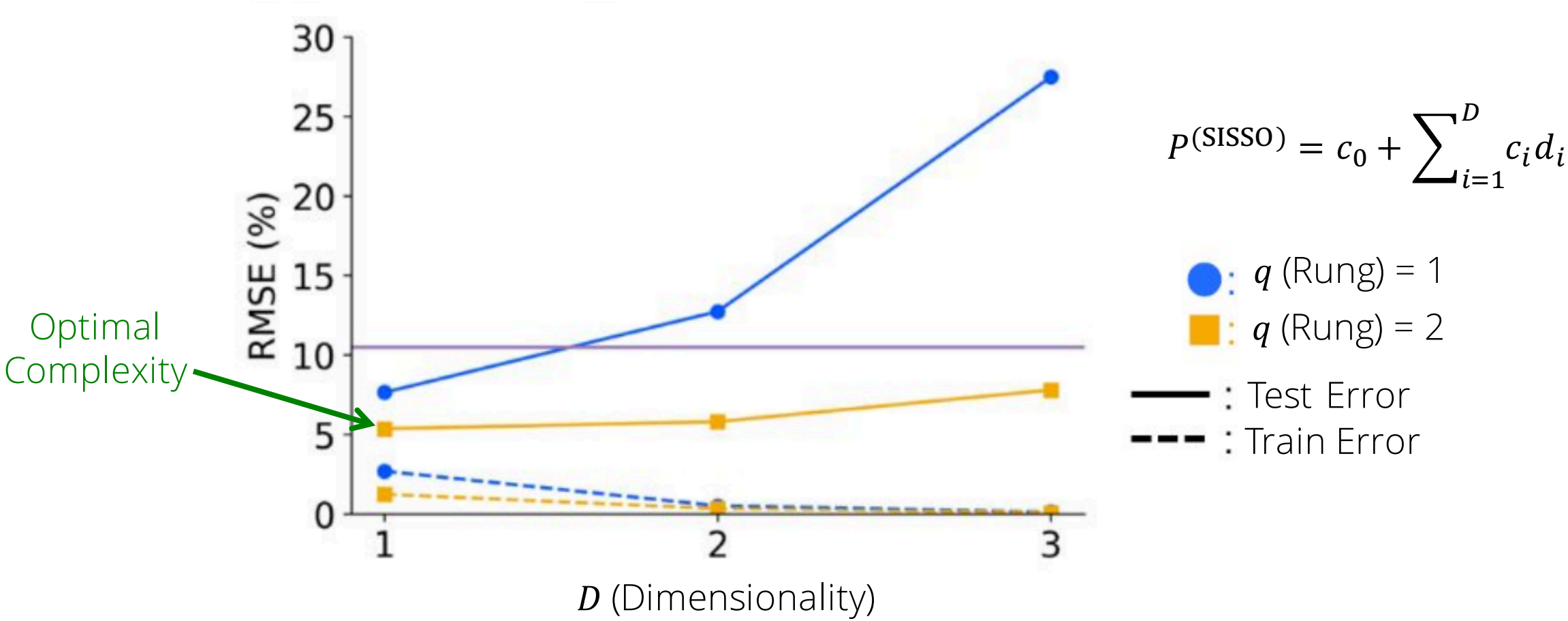
- Experiment
- Calculation

33 Candidate Descriptive Parameters

R. Miyazaki *et al.* JACS 146, 5433 (2024)

Application: Describing the Performance of Silica-Supported Cobalt Catalysts (Co/*M*-SiO_2) in CO_2 Hydrogenation

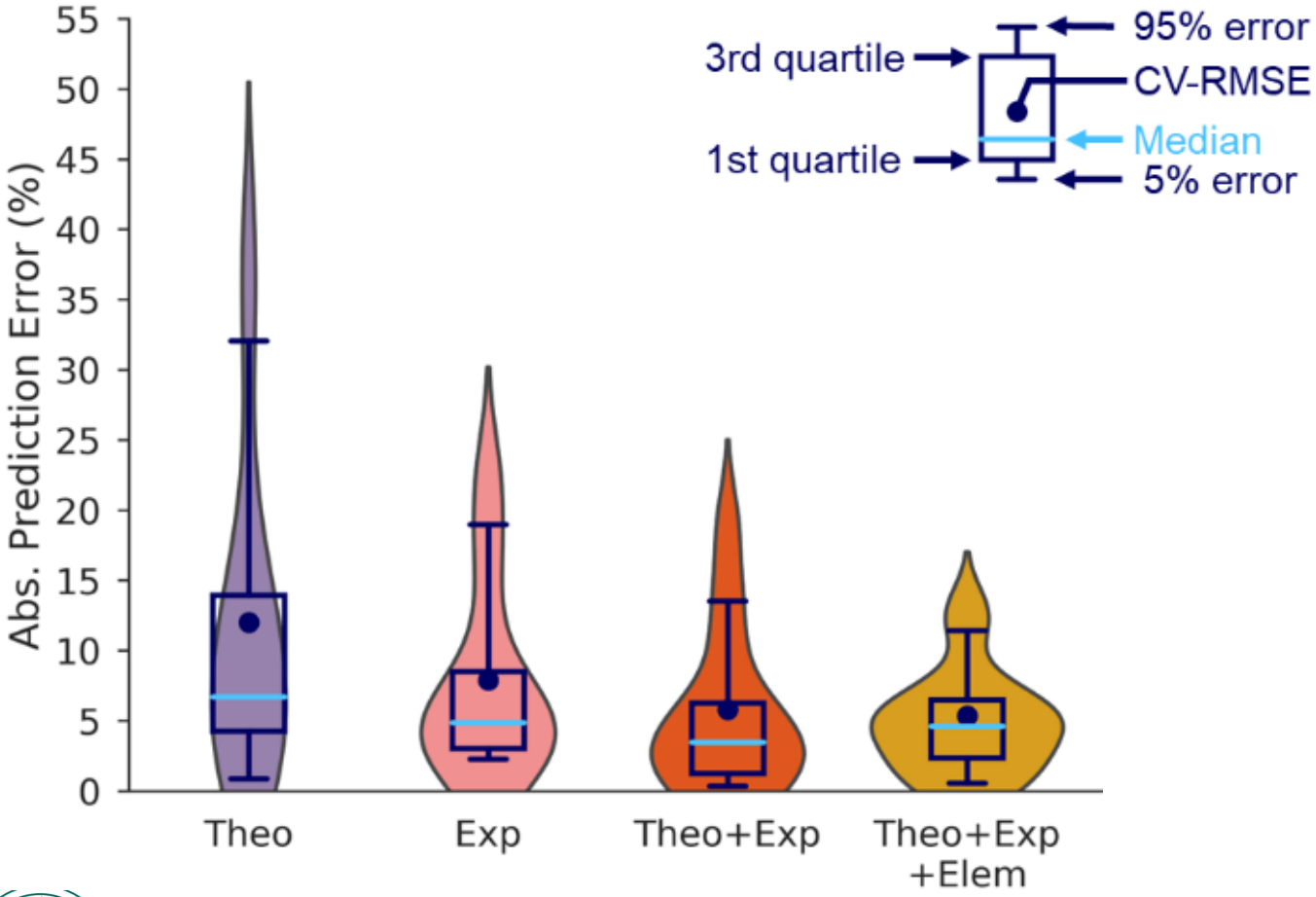
Determination of SISSO Model Hyperparameters (Leave-One-Material-Out Cross Validation)



R. Miyazaki *et al.* JACS 146, 5433 (2024)

Application: Describing the Performance of Silica-Supported Cobalt Catalysts (Co/*M*-SiO_2) in CO_2 Hydrogenation

Error Distributions Associated to SISSO Models for Methanol Selectivity



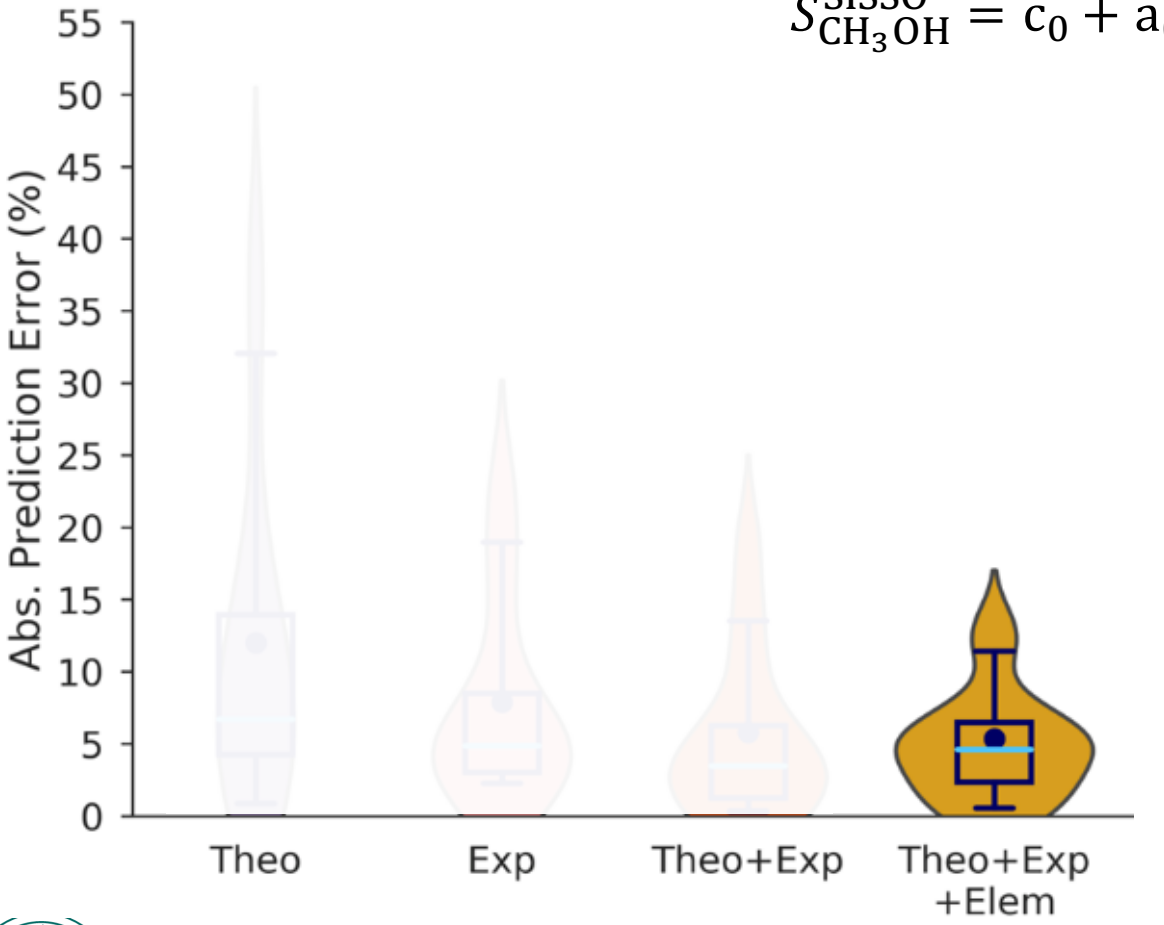
- Improved Description Combining Theoretical (Theo), Experimental (Exp), and Elemental (Elem) Primary Features

R. Miyazaki *et al.* JACS 146, 5433 (2024)

Application: Describing the Performance of Silica-Supported Cobalt Catalysts (Co/*M*-SiO_2) in CO_2 Hydrogenation

CO_2 Conversion (Exp)

$$S^{\text{SISSO}}_{\text{CH}_3\text{OH}} = c_0 + a_0 \left\{ \frac{M_{\text{cov}} * X^{RGSV}_{CO2}}{E_{CH3O} * T_{H2}} \right\}$$



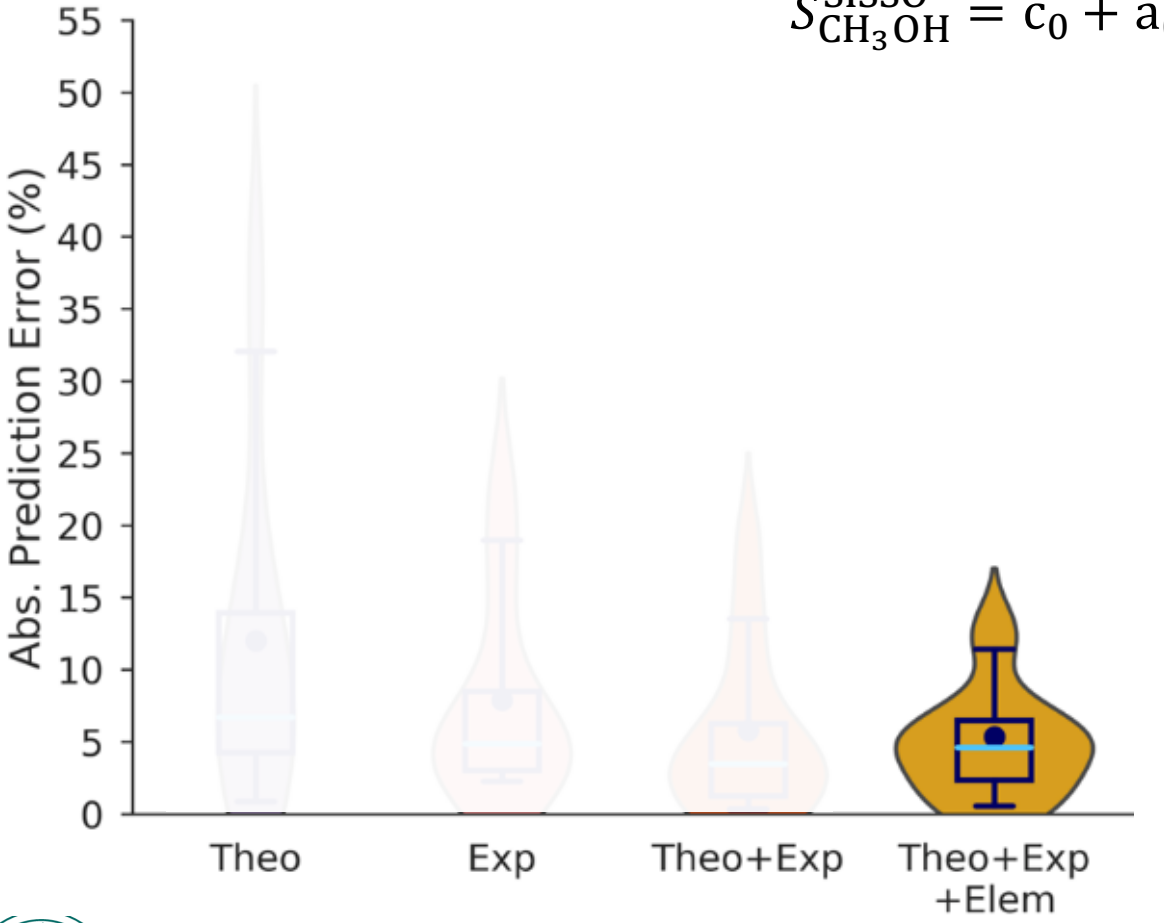
R. Miyazaki *et al.* JACS 146, 5433 (2024)

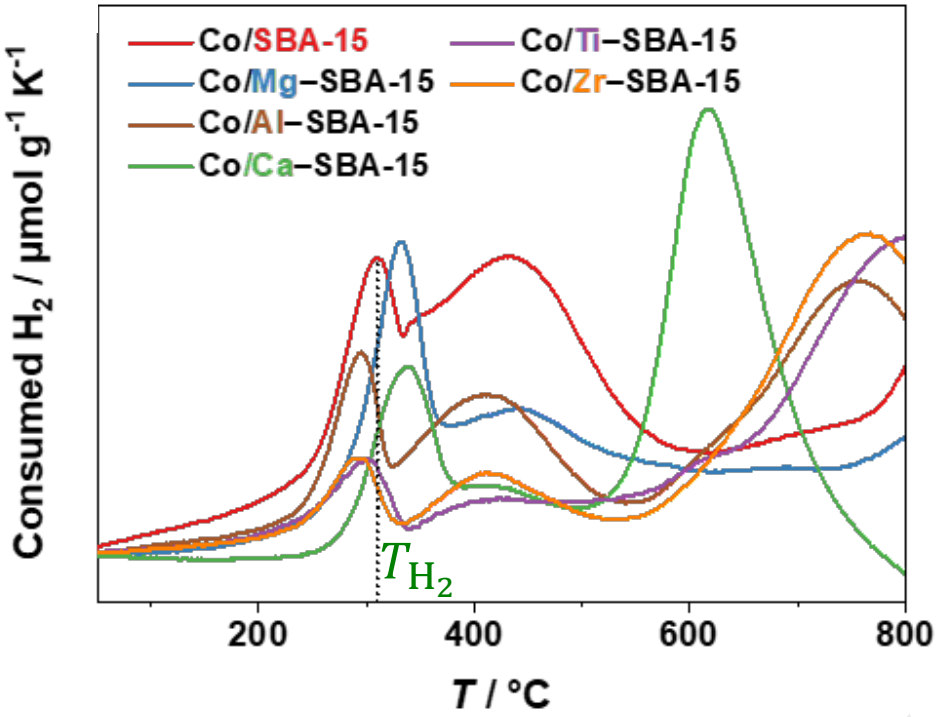
Application: Describing the Performance of Silica-Supported Cobalt Catalysts (Co/*M*-SiO_2) in CO_2 Hydrogenation

$$S_{CH_3OH}^{SISSO} = c_0 + a_0 \left\{ \frac{M_{cov} * X_{CO2}^{RGSV}}{E_{CH3O} * T_{H2}} \right\}$$

CO_2 Conversion (Exp)

Temperature of 1st H_2-TPR Signal (Exp)





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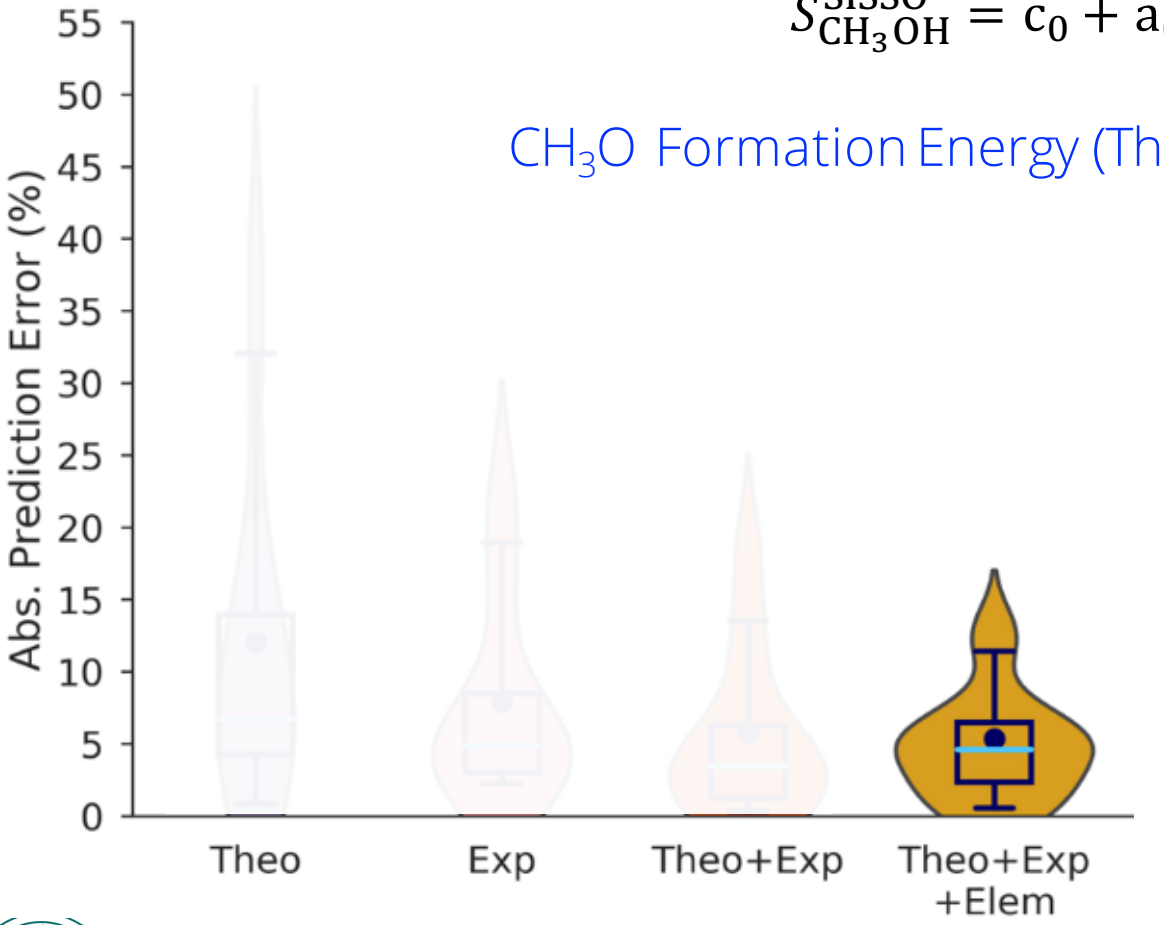
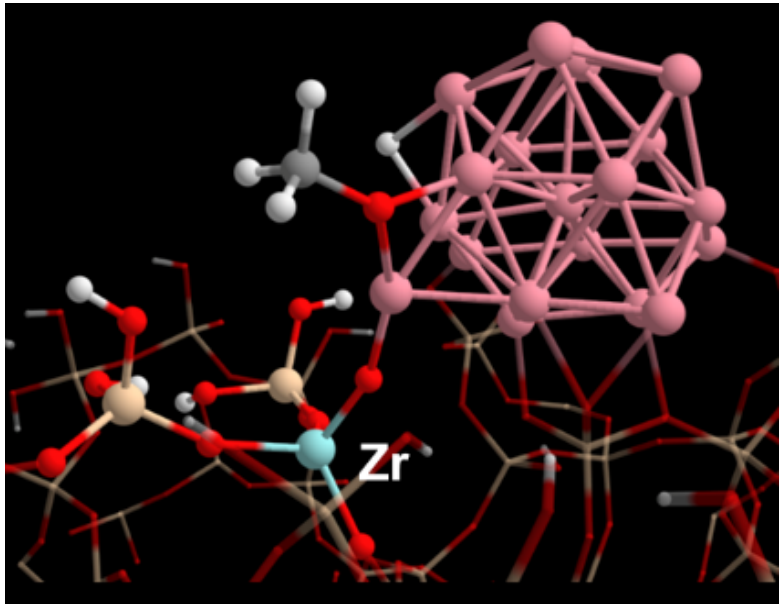
CO_2 Conversion (Exp)

CH_3O Formation Energy (Theo)

Temperature of 1st H_2-TPR Signal (Exp)



M	E_{CH_3O}(eV)
-	-1.49
Ti	-1.50
Zr	**-1.39**
Al	-0.97
Ca	-1.13
Mg	-1.55



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Application: Describing the Performance of Silica-Supported Cobalt Catalysts (Co/*M*-SiO_2) in CO_2 Hydrogenation

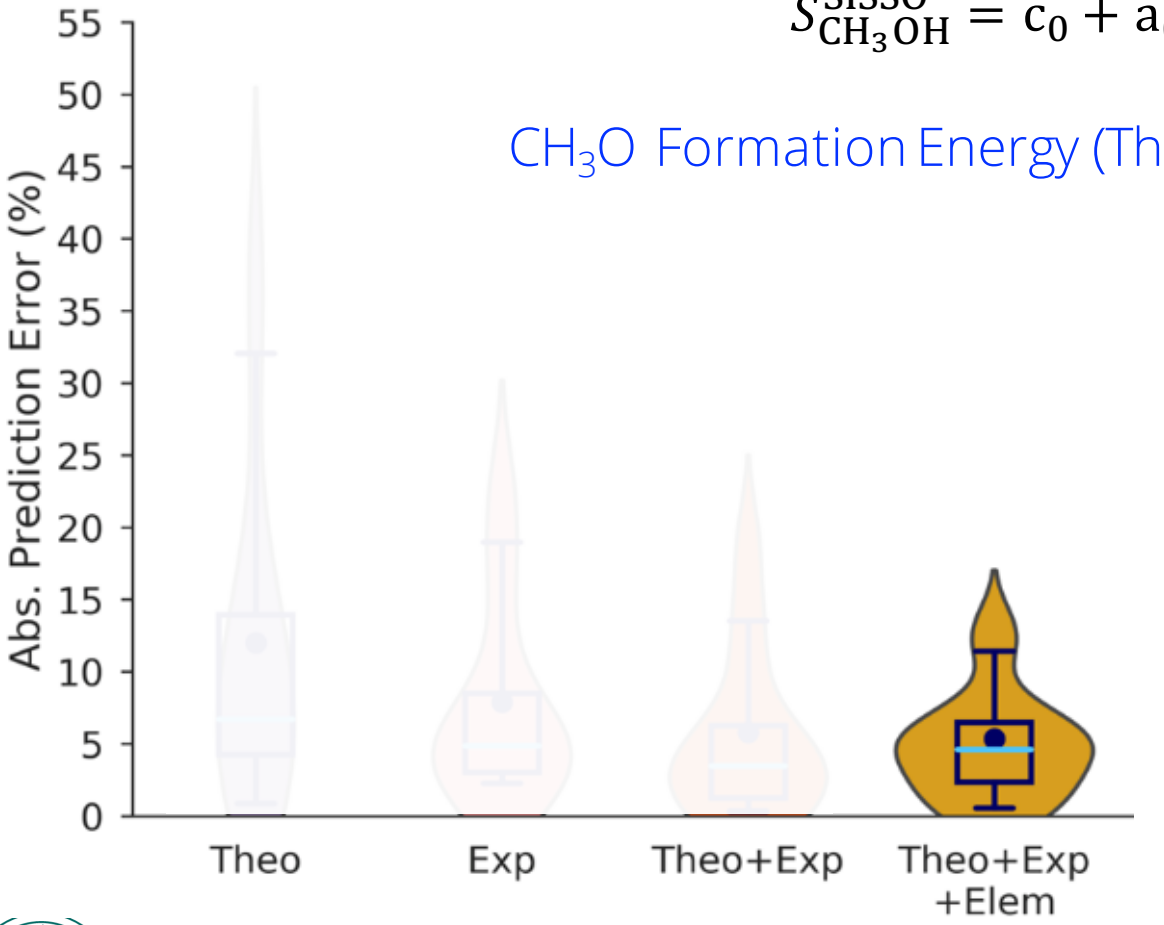
M Covalent Atomic Radius (Elem)

CO_2 Conversion (Exp)

$$S^{\text{SISSO}}_{\text{CH}_3\text{OH}} = c_0 + a_0 \left\{ \frac{M_{\text{cov}} * X^{RGSV}_{CO2}}{E_{CH3O} * T_{H2}} \right\}$$

CH_3O Formation Energy (Theo)

Temperature of 1st H_2-TPR Signal (Exp)



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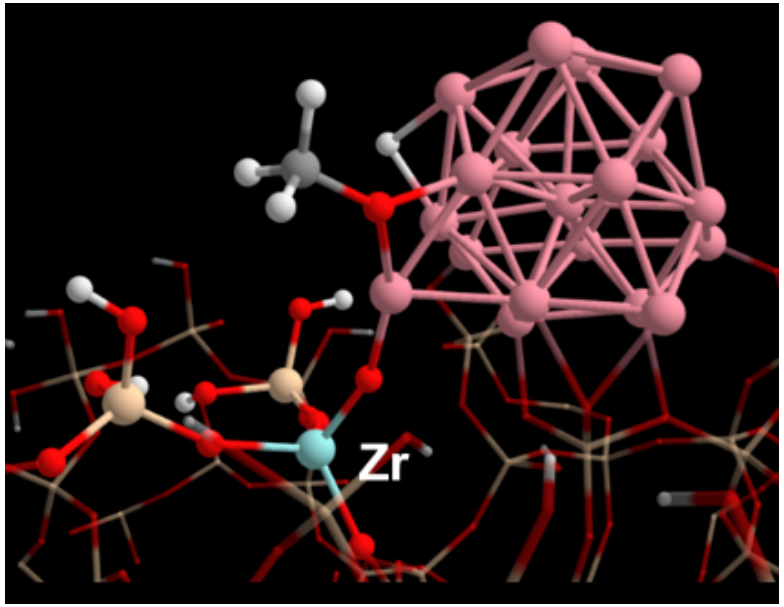

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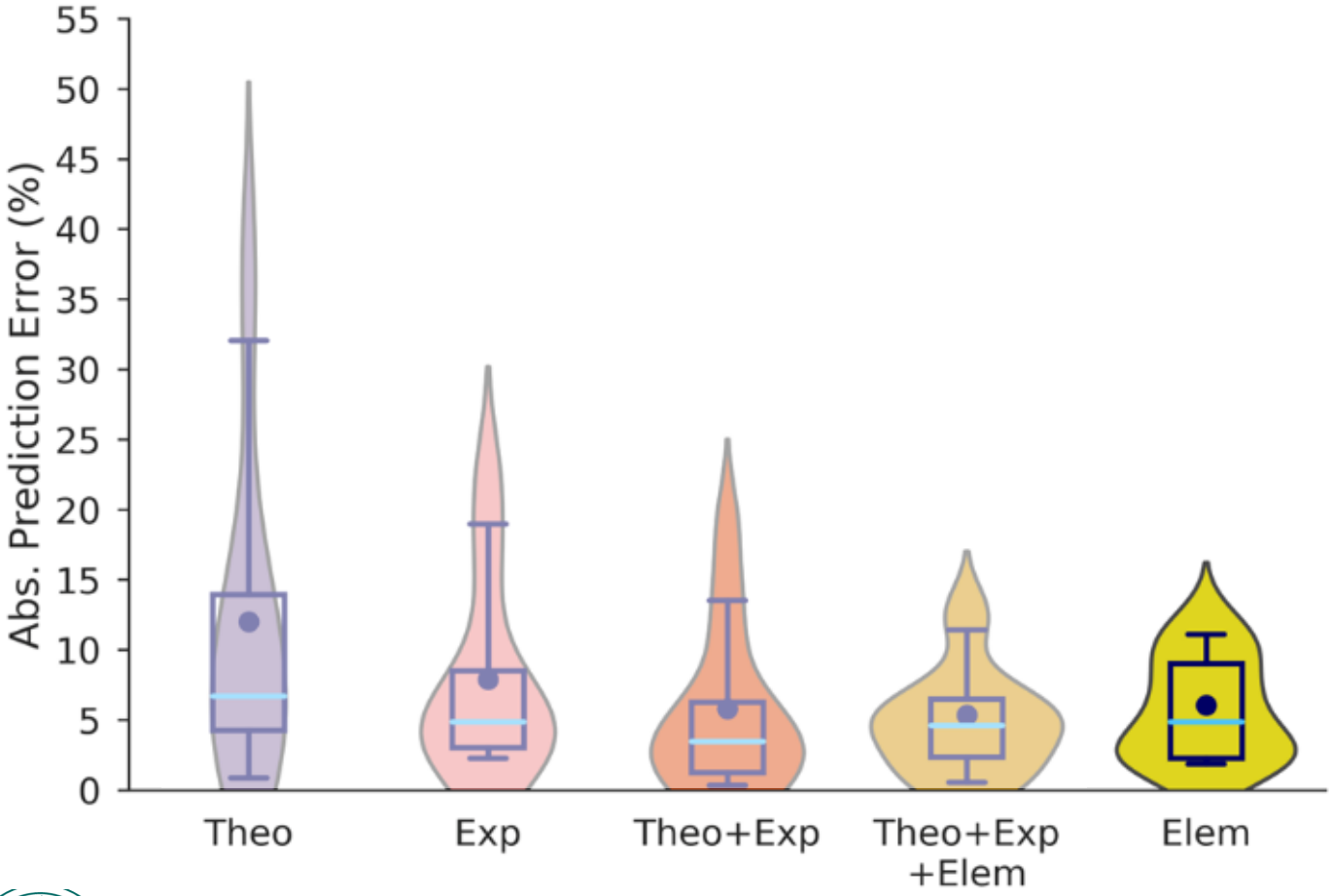
Application: Describing the Performance of Silica-Supported Cobalt Catalysts (Co/*M*-SiO_2) in CO_2 Hydrogenation

SISSO Model Based Only on Elemental Parameters Suggests New Supports



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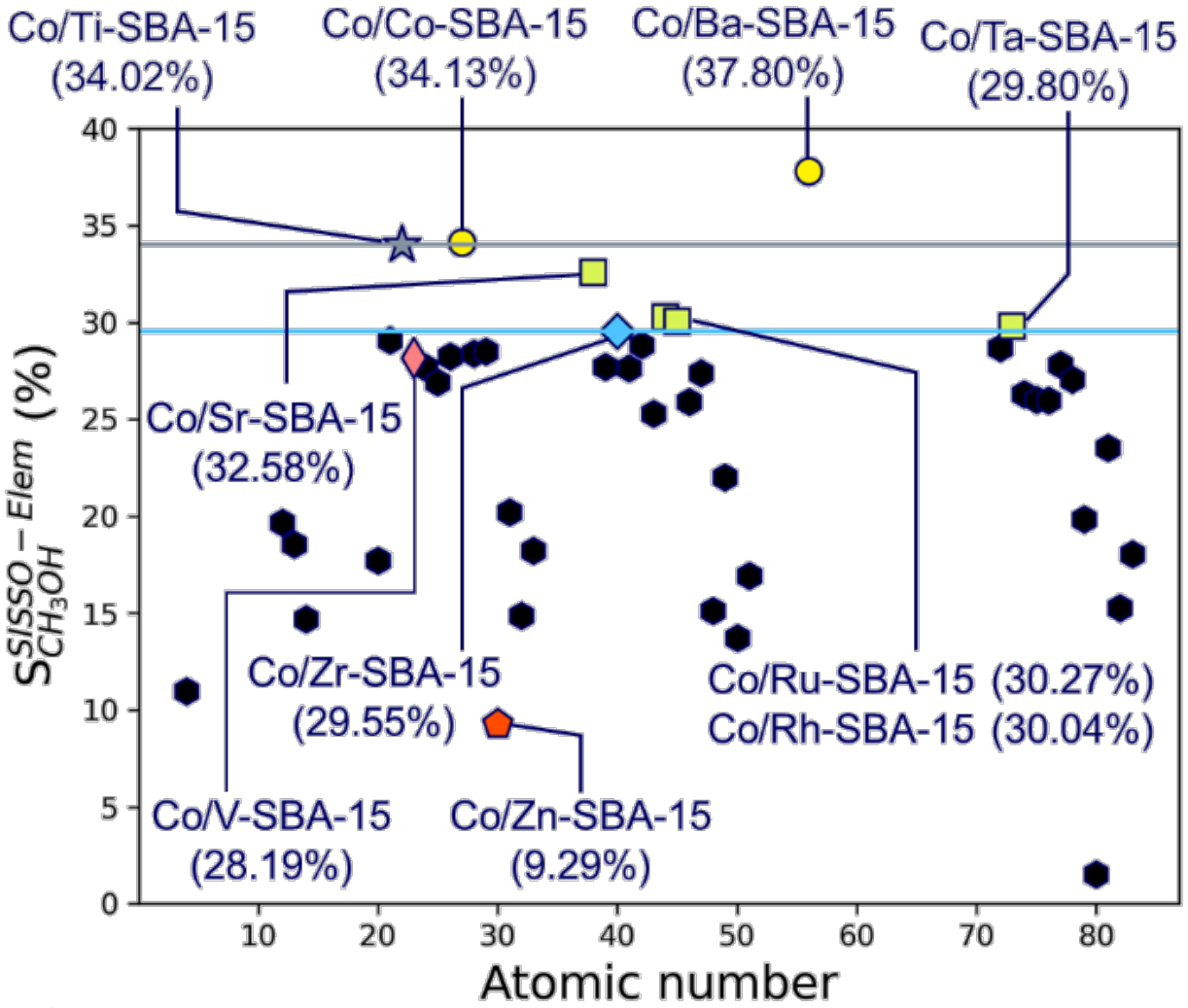

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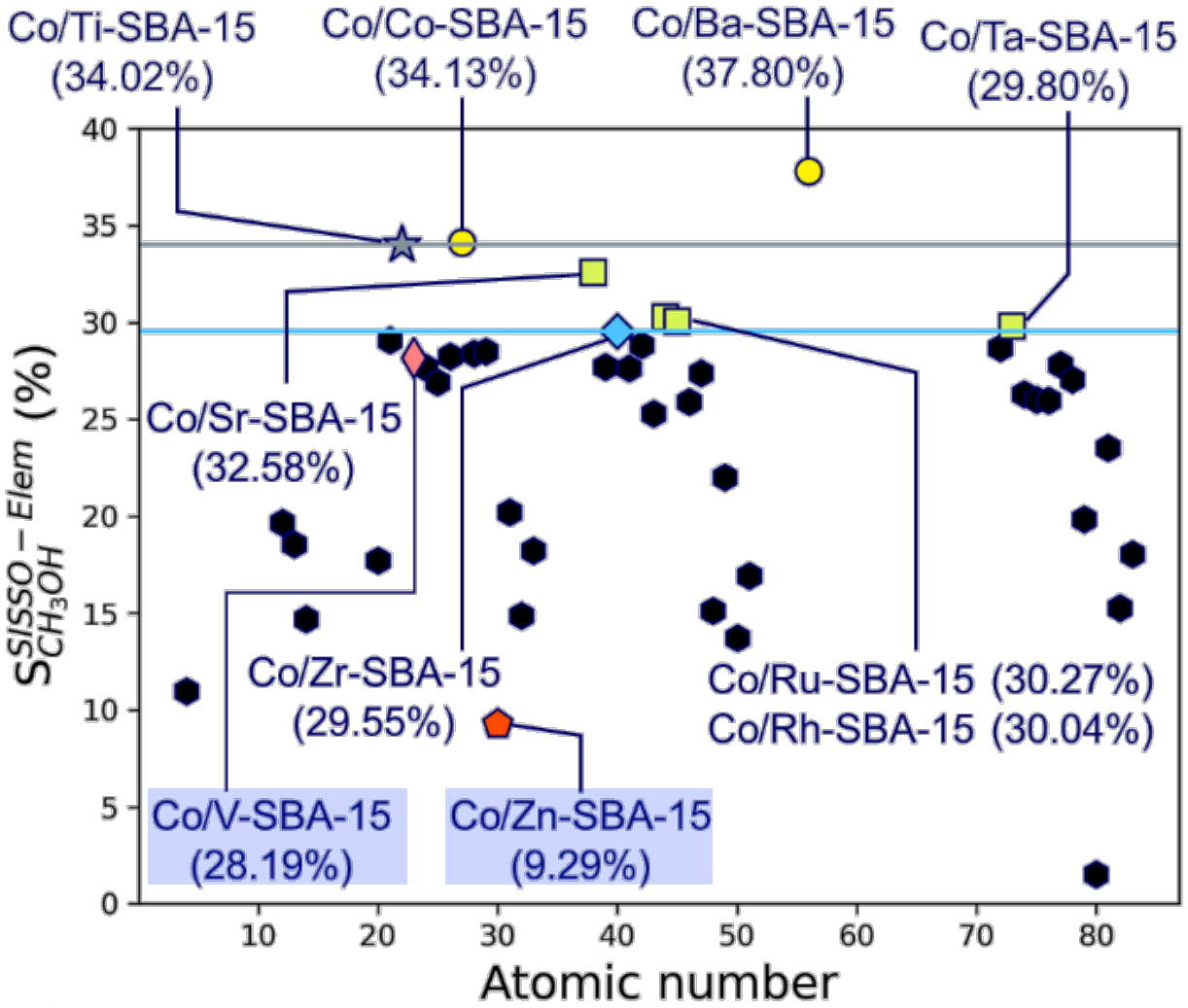

SISSO Model Based Only on Elemental Parameters Suggests New Supports

material	$S^{\mathrm{SISSO}}_{\mathrm{CH_3OH}}$ (predicted)	$\sigma^{\mathrm{SISSO}}_{S_{\mathrm{CH_3OH}}}$
Co/**V**-SiO_2	28.19	3.9
Co/**Zn**–SiO_2	9.29	20.6

↑ Standard Deviation of Predictions of SISSO Models

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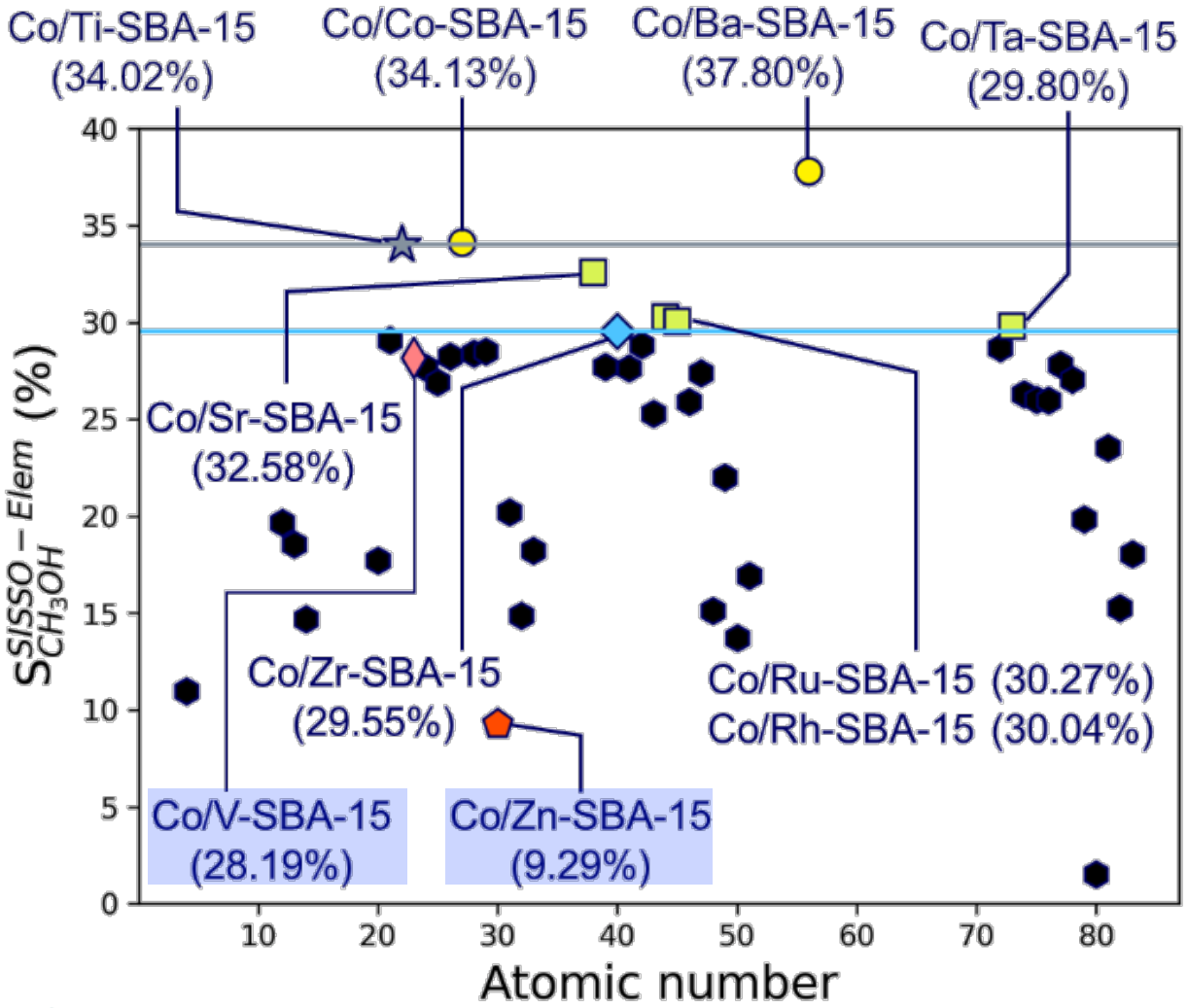

SISSO Model Based Only on Elemental Parameters Suggests New Supports

material	$S^{SISSO}_{CH_3OH}$ (predicted)	$\sigma^{SISSO}_{S_{CH_3OH}}$	$S^{exp}_{CH_3OH}$ (measured)
Co/**V**-SiO_2	28.19	3.9	32.5
Co/**Zn**–SiO_2	9.29	20.6	16.9

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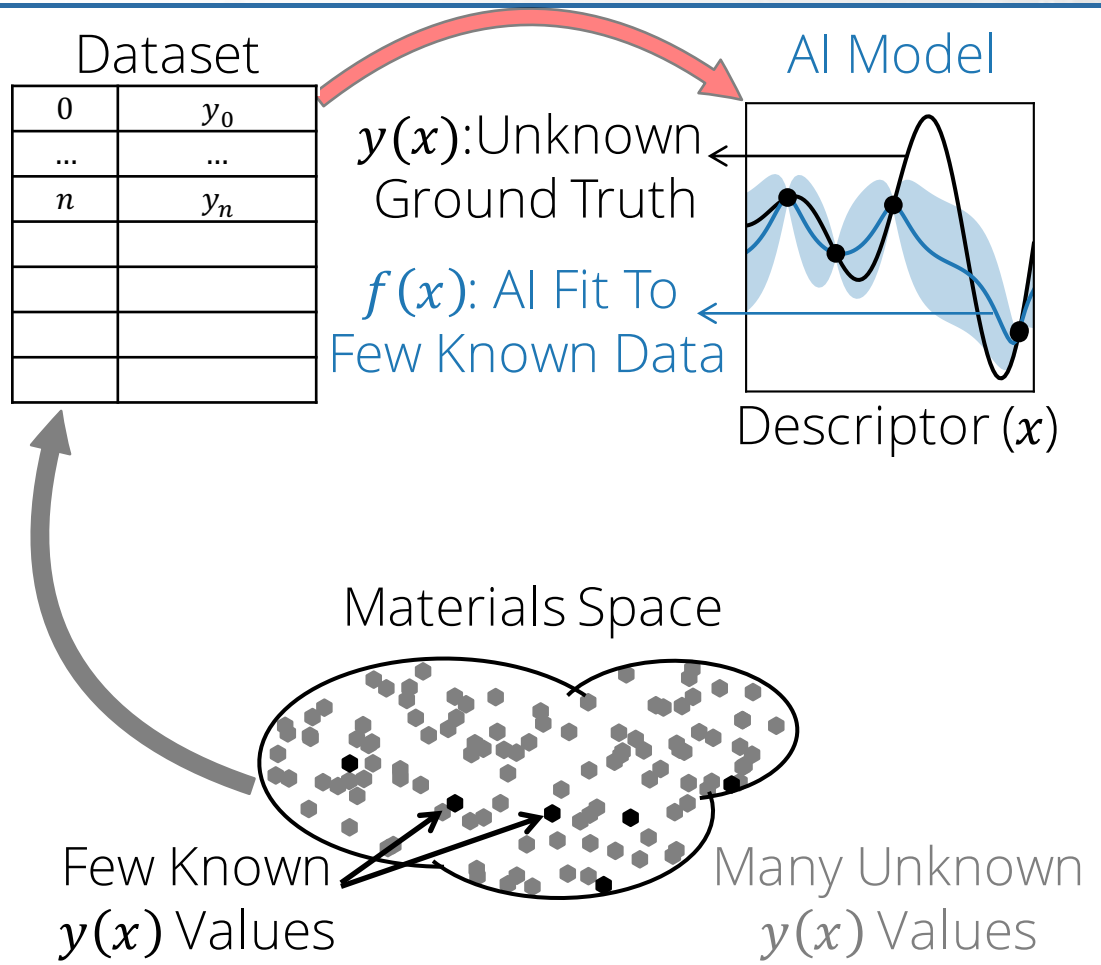
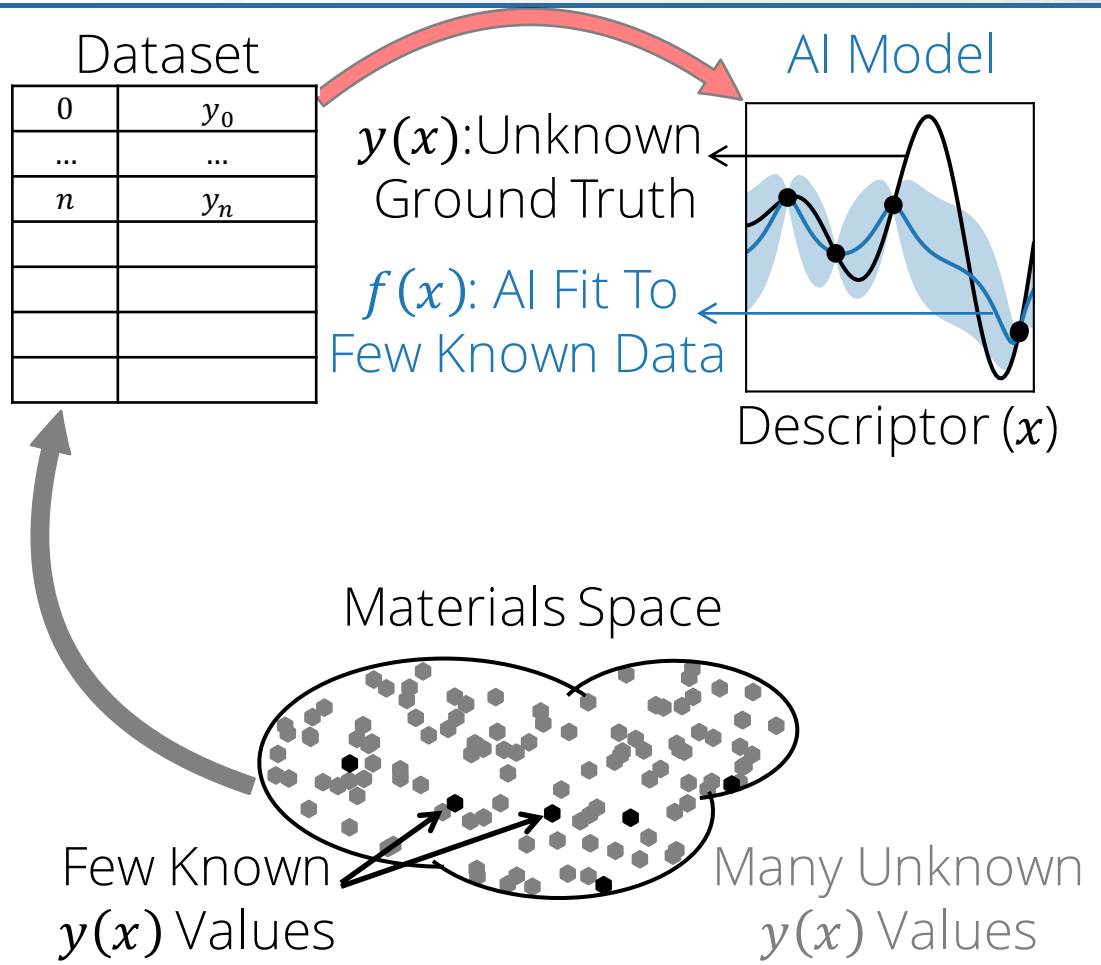
AI Models of Materials Properties



AI Models of Materials Properties

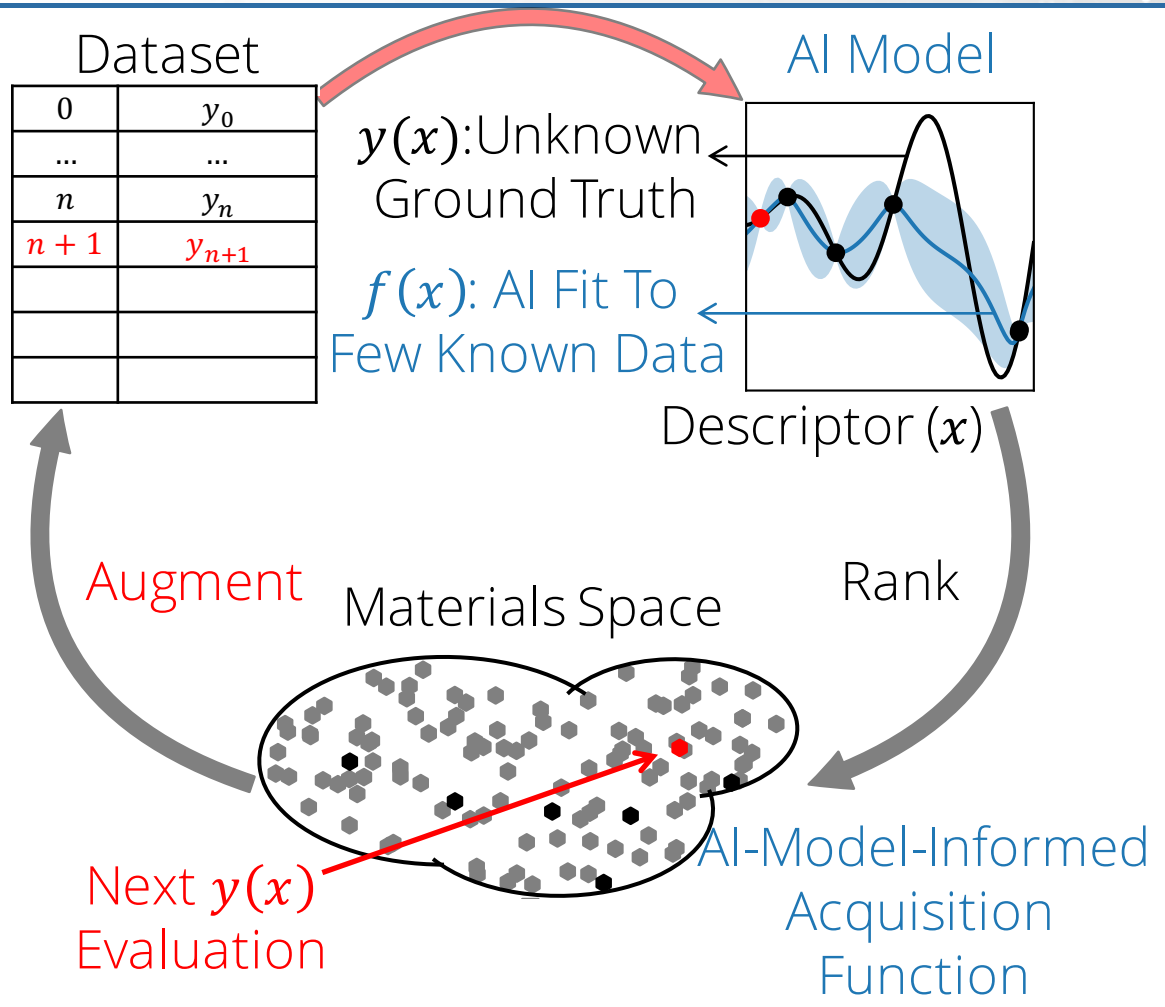
- Model Performance Assessed in Average
- Good Average Performance Might Not Translate to Good Description of Promising Materials



S. Kauwe *et al.*, Comput. Mat. Sci. 174, 109498 (2020)
B. Meredig *et al.*, Mol. Syst. Des. Eng. 3, 819 (2018)

From Prediction to Action: AI-Guided Workflows for the Discovery of Materials with Optimal Properties

- Iterative Modelling and Data Acquisition Approach to Identify Materials with Desired Property Values (e.g., High)



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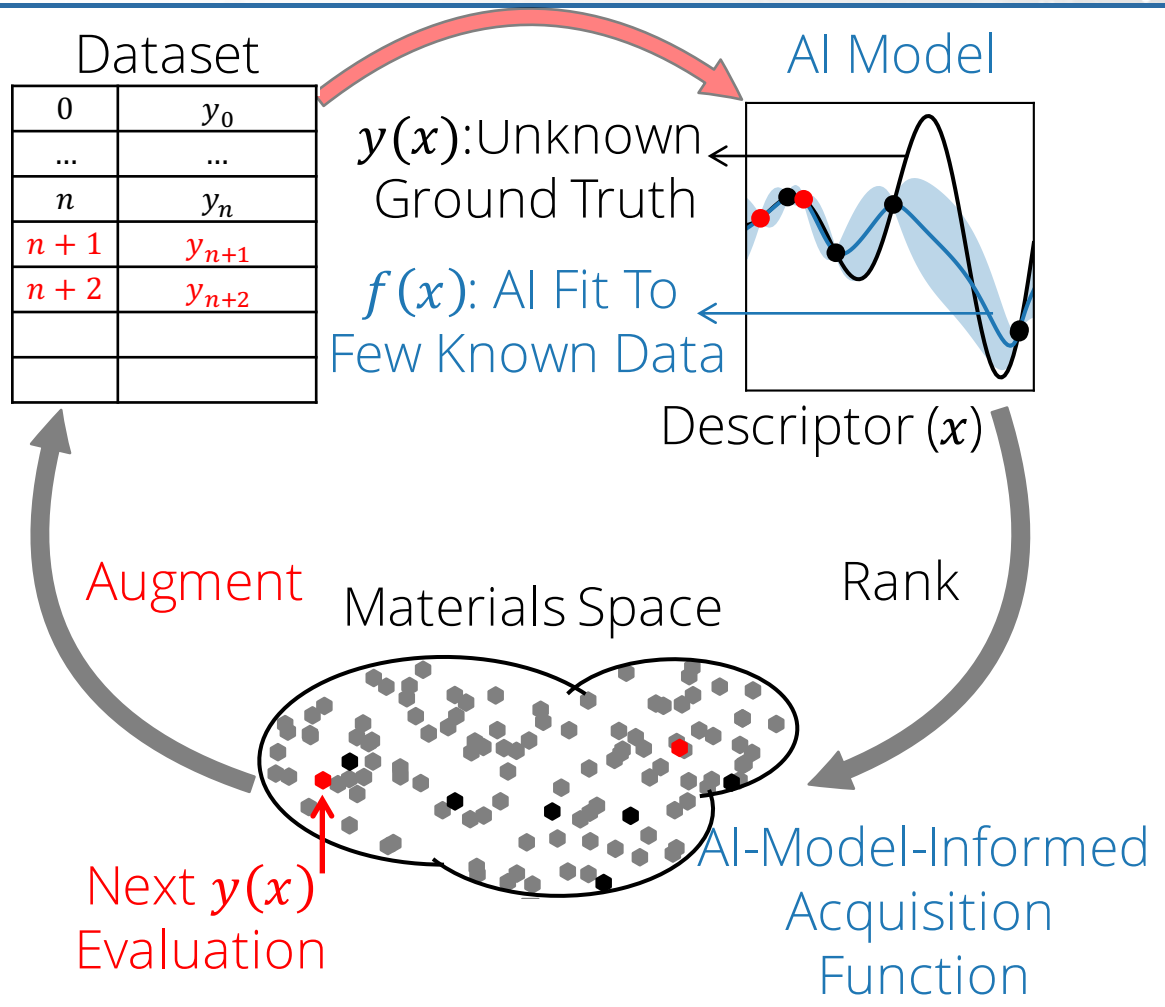

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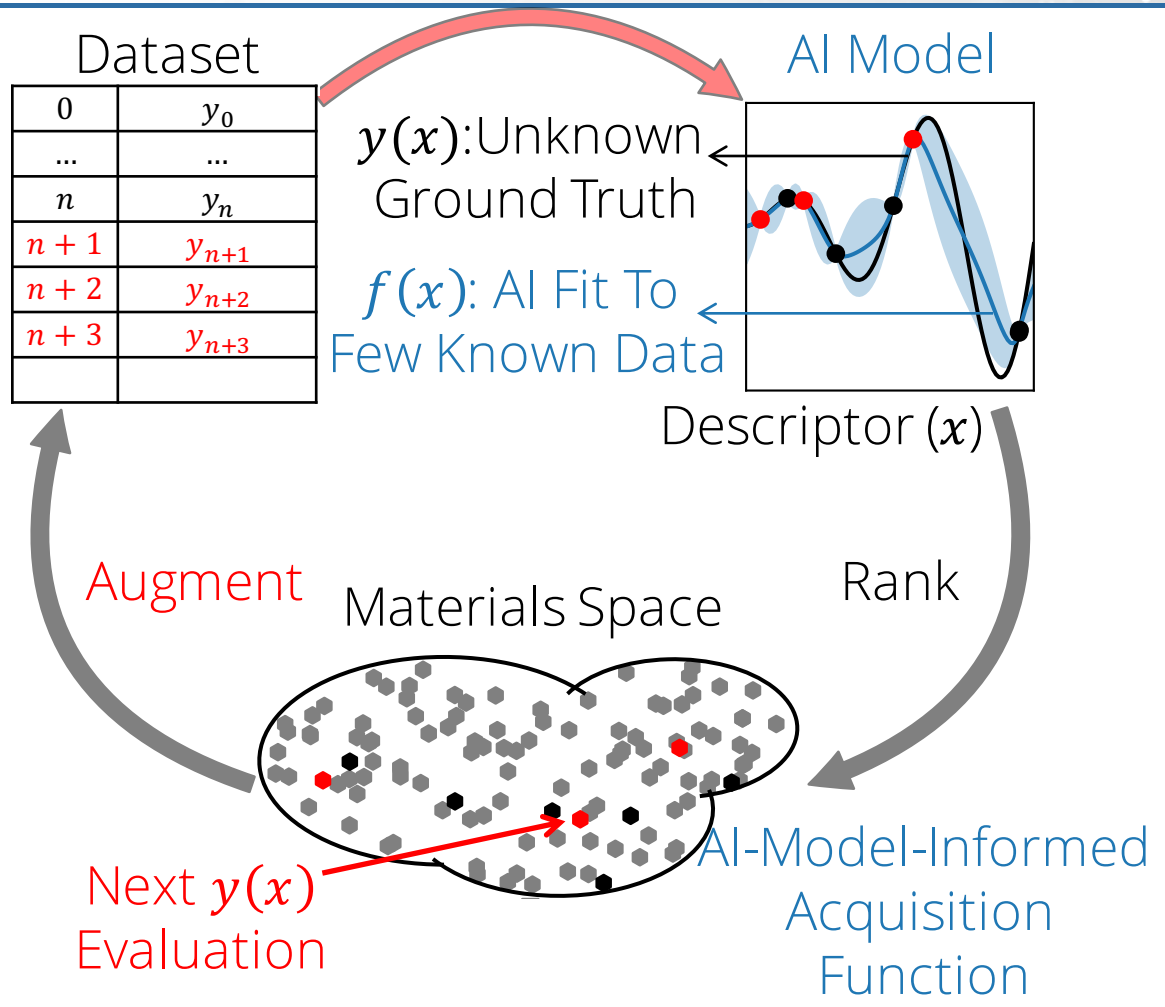

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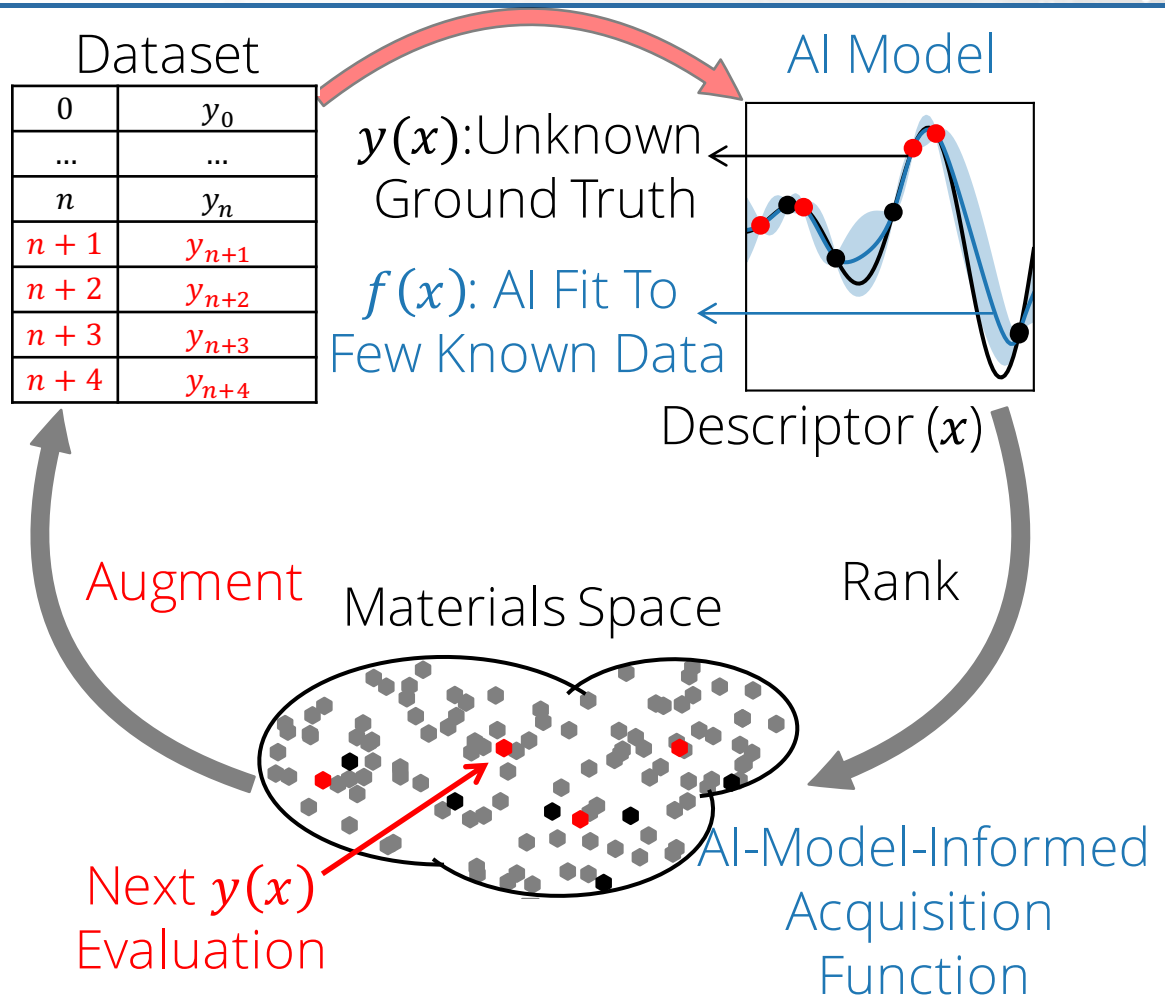

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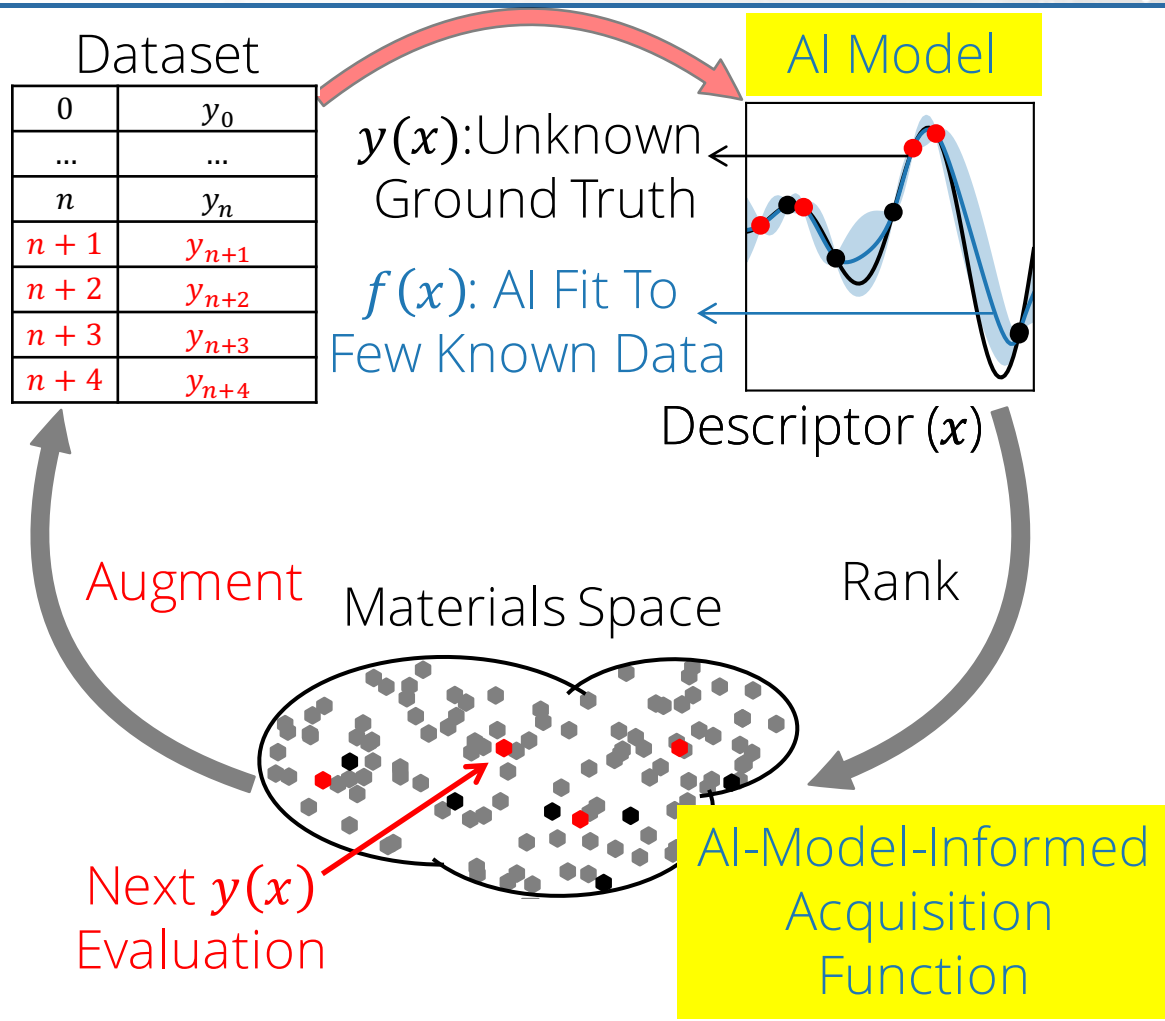
1. Impact of Choices of AI Model and Acquisition Function?



0	y_0
...	...
n	y_n
$n+1$	y_{n+1}
$n+2$	y_{n+2}
$n+3$	y_{n+3}
$n+4$	y_{n+4}

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From Prediction to Action: AI-Guided Workflows for the Discovery of Materials with Optimal Properties

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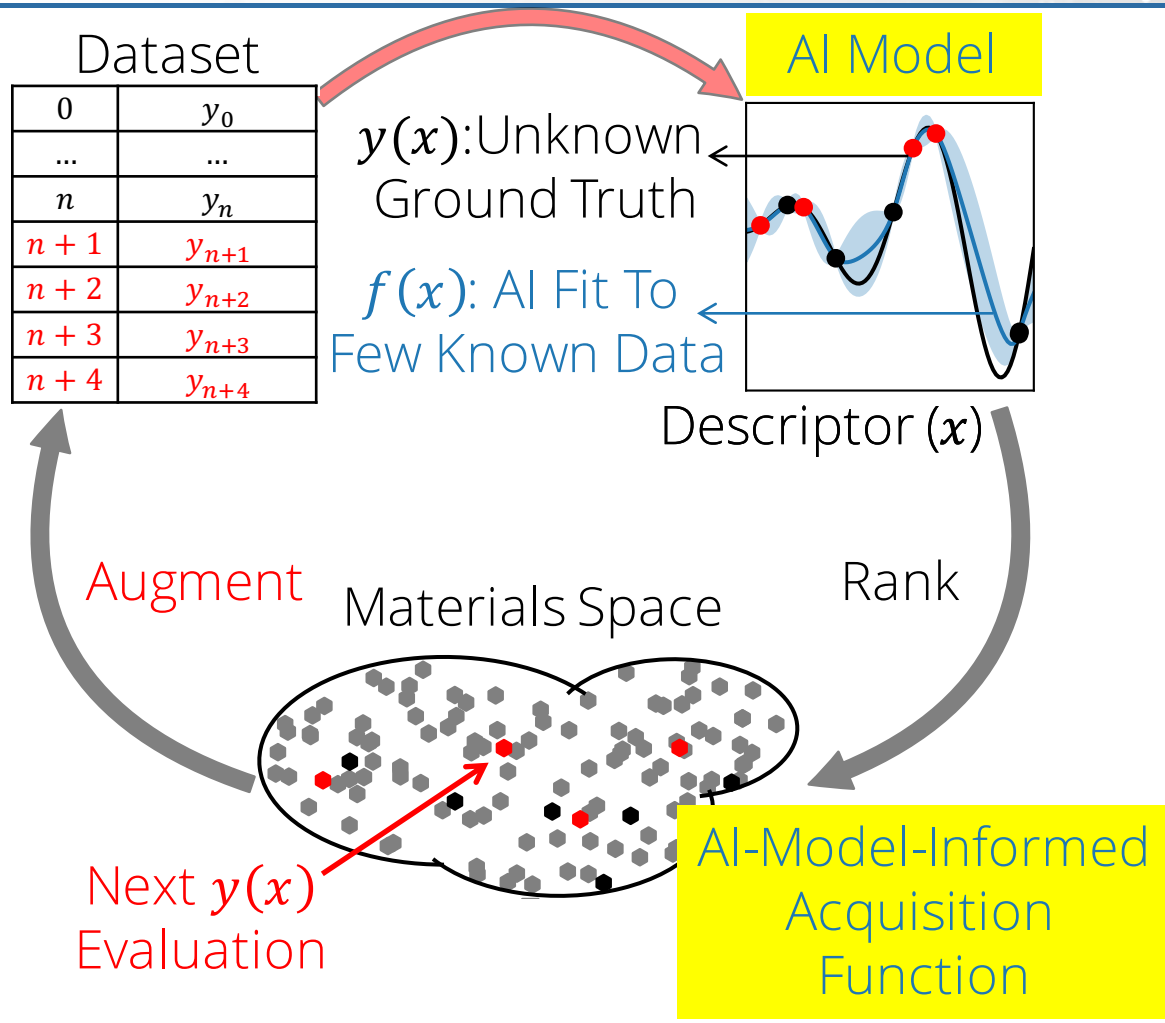
1. Impact of Choices of AI Model and Acquisition Function?

2. SISSO-Guided Workflow?



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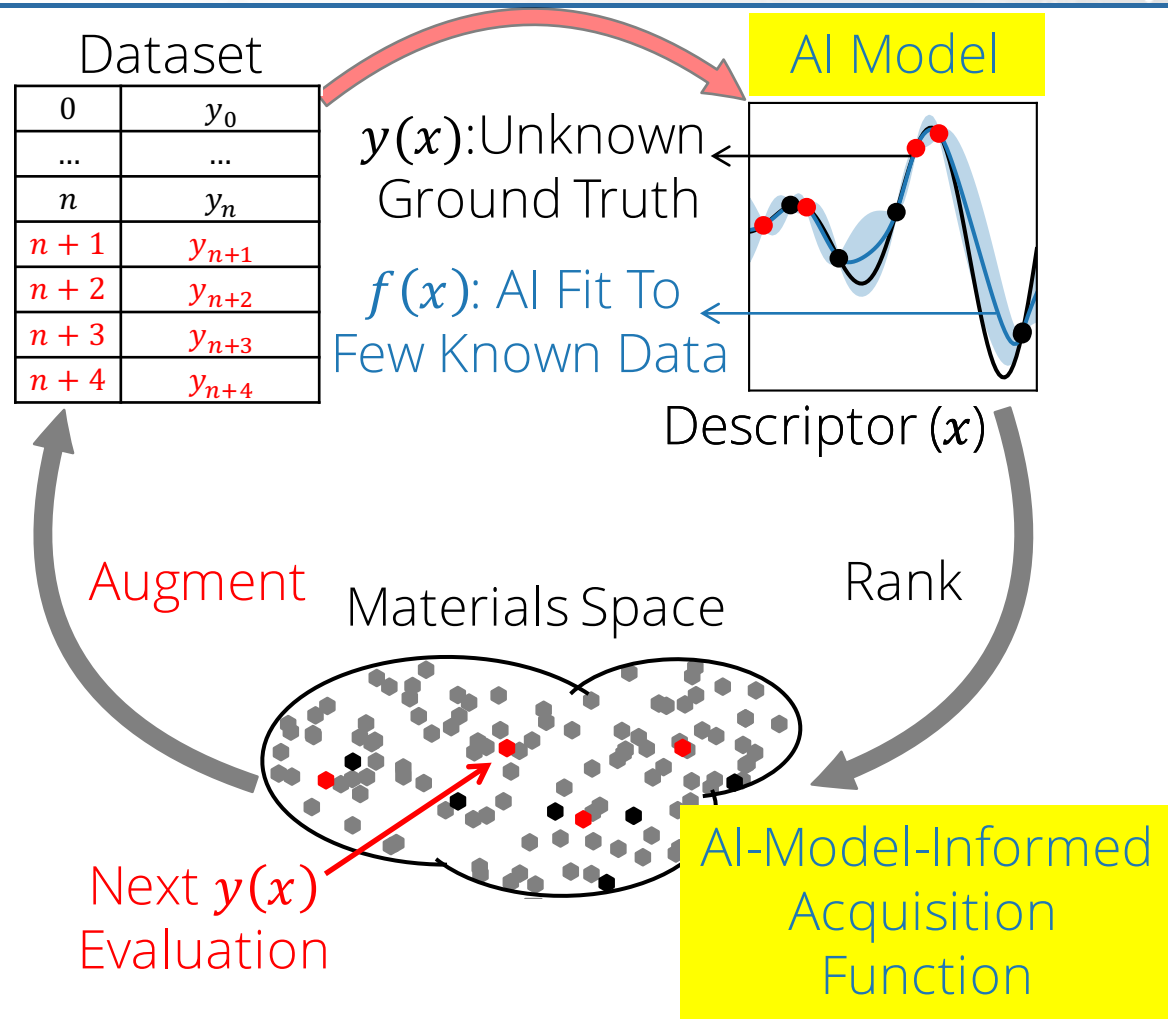
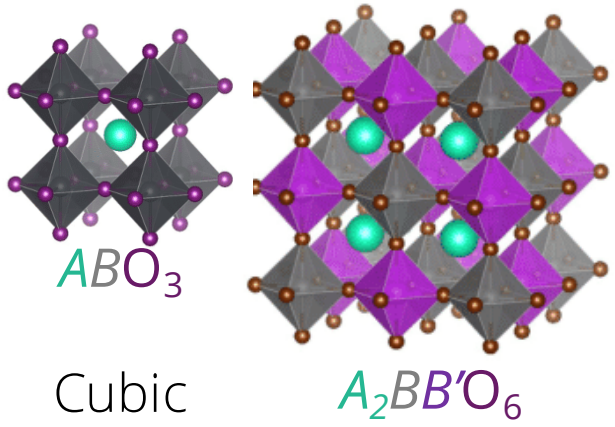
2. SISSO-Guided Workflow?

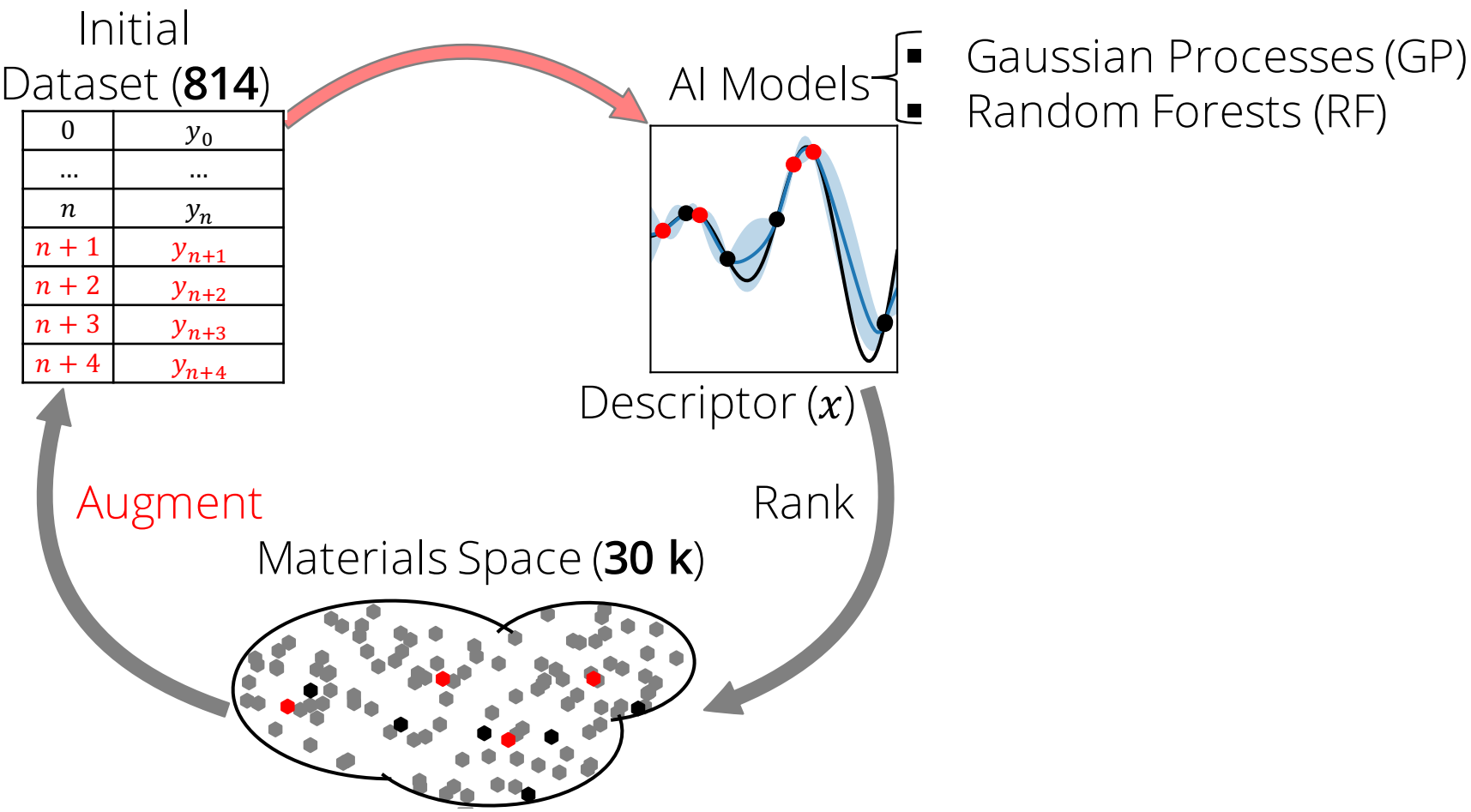


B. Shahriari *et al.*, Proc. IEEE, 104, 1 148 (2016)

Workflow 1: Identifying Perovskites with High Bulk Modulus

- Target Property (y):
  Bulk Modulus (B_0)





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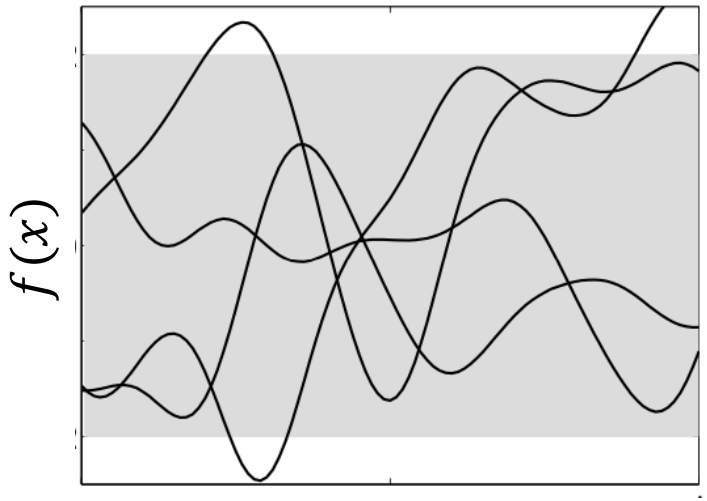
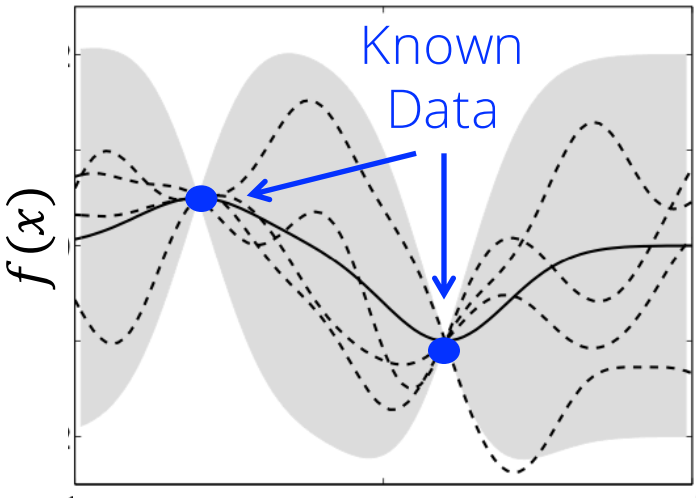
Gaussian Processes (GP)

- Probabilistic Model Providing Mean Predictions and Confidence Intervals (Uncertainty)
  - Learns a Distribution Over All Possible Functions that Fit the Data





Prior Distribution

- Distribution of Functions Generated Using Assumptions on Continuity and Smoothness (Kernel)
- All Functions Are Possible Before Seeing Data

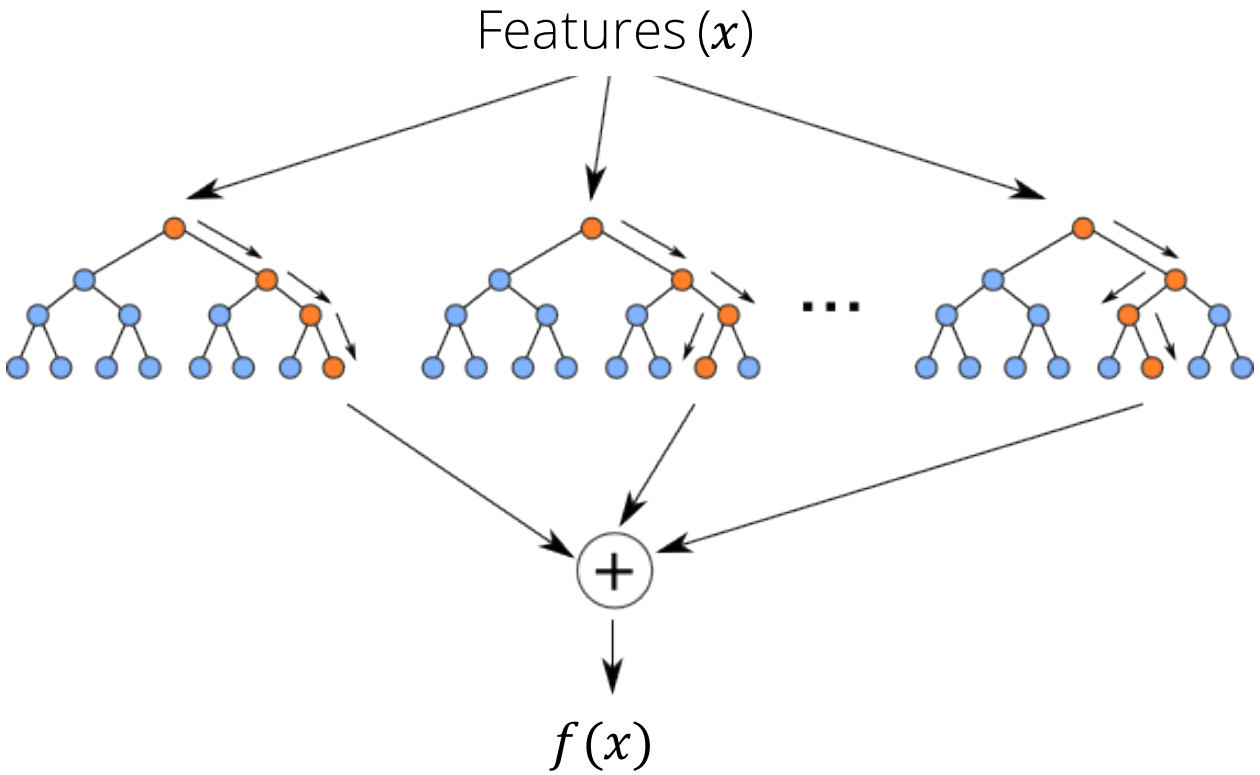
Posterior Distribution

- After Seeing Data, Some Functions Become More Important than Others

Random Forests (RFs)

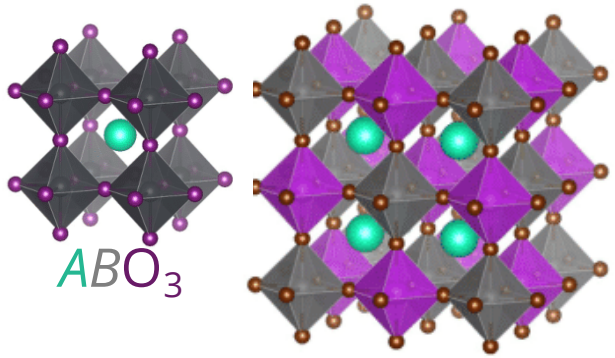
- Combines the Predictions of Many (Ensemble) of Decision Trees, Each Trained on a Subset of Data and Features

- Variability of Predictions Across Trees Estimates Prediction Uncertainty



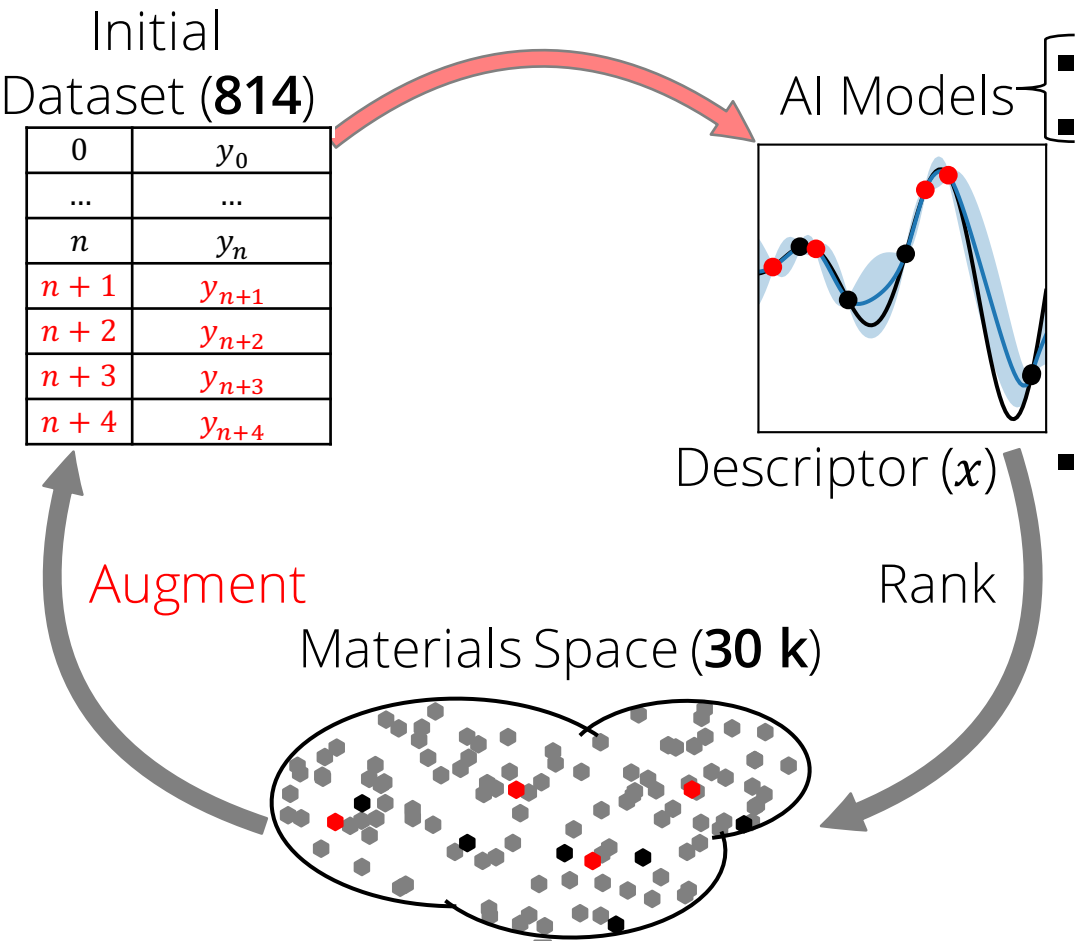
Workflow 1: Identifying Perovskites with High Bulk Modulus

- Target Property (y):
  Bulk Modulus (B_0)



ABO_3 Cubic

$A_2BB'O_6$



- Gaussian Processes (GP)
- Random Forests (RF)

- Elemental Properties of ***A*** and ***B*** (e.g. Radii, Electronegativity, Ionization Potential)

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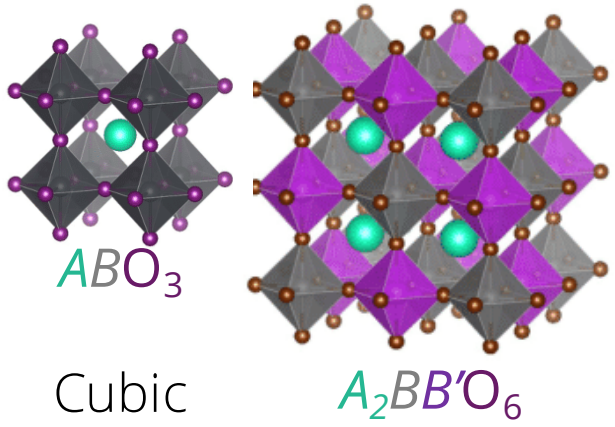
Workflow 1: Identifying Perovskites with High Bulk Modulus

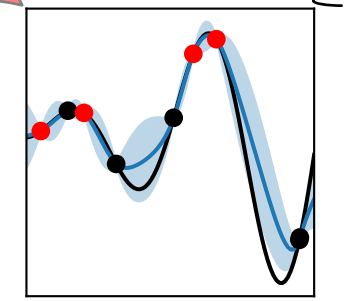
- Target Property (y):
  Bulk Modulus (B_0)



Initial Dataset (**814**)

0	y_0
...	...
n	y_n
$n+1$	y_{n+1}
$n+2$	y_{n+2}
$n+3$	y_{n+3}
$n+4$	y_{n+4}

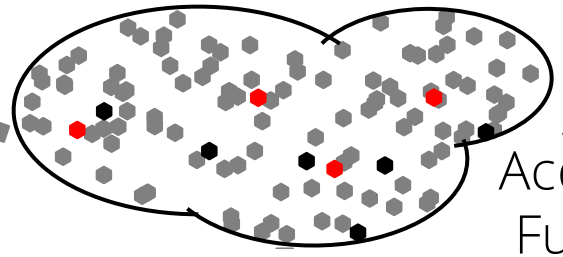
AI Models
- Gaussian Processes (GP)
- Random Forests (RF)



Descriptor (x)
- Elemental Properties of ***A*** and ***B*** (e.g. Radii, Electronegativity, Ionization Potential)

Rank

Materials Space (**30 k**)



Augment

Acquisition Functions
- Pure Exploitation (XT)
- Expected Improvement (EI)

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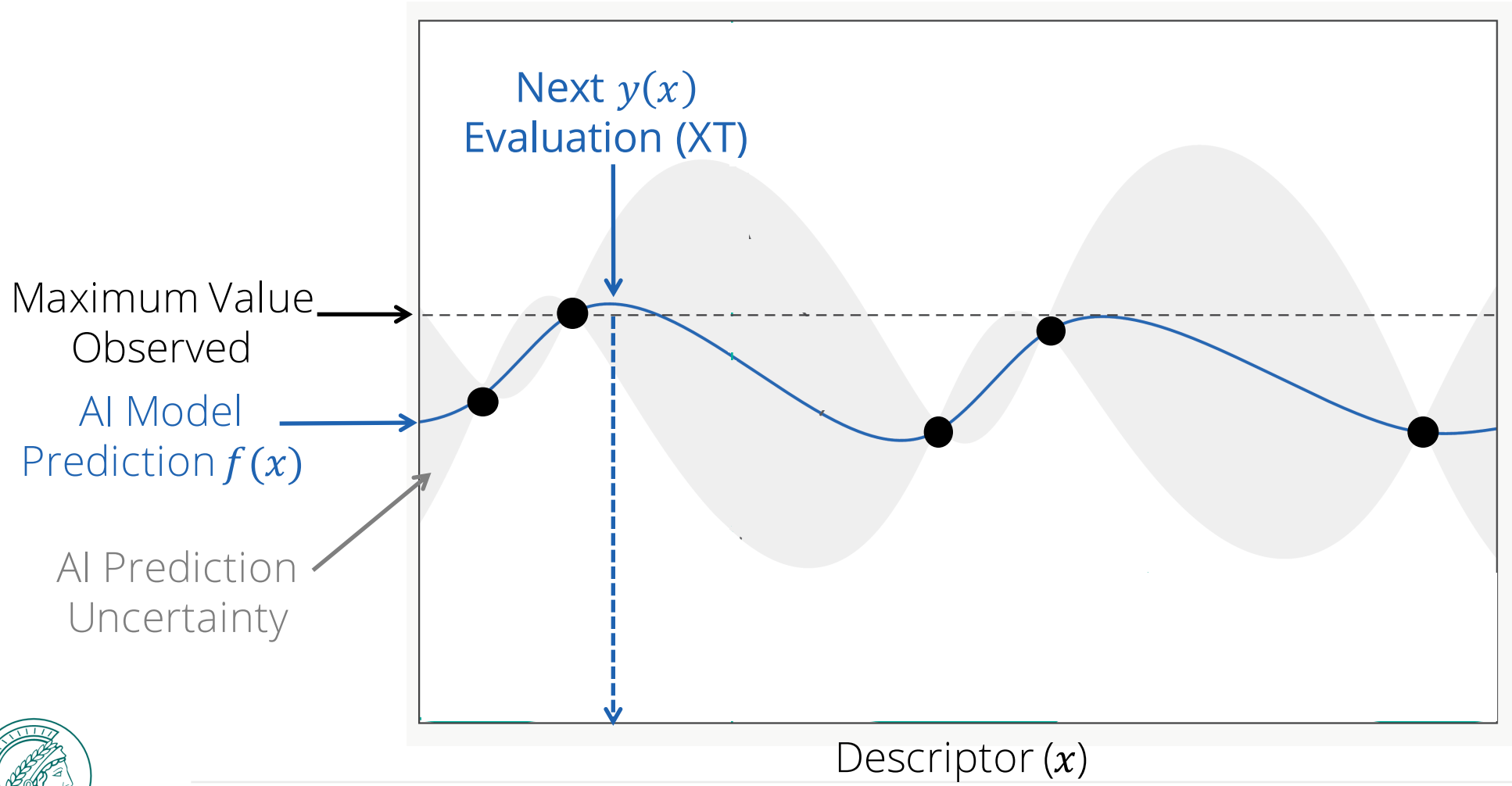
Workflow 1: Identifying Perovskites with High Bulk Modulus

- **Reward:** Maximum B_0 Observed So Far

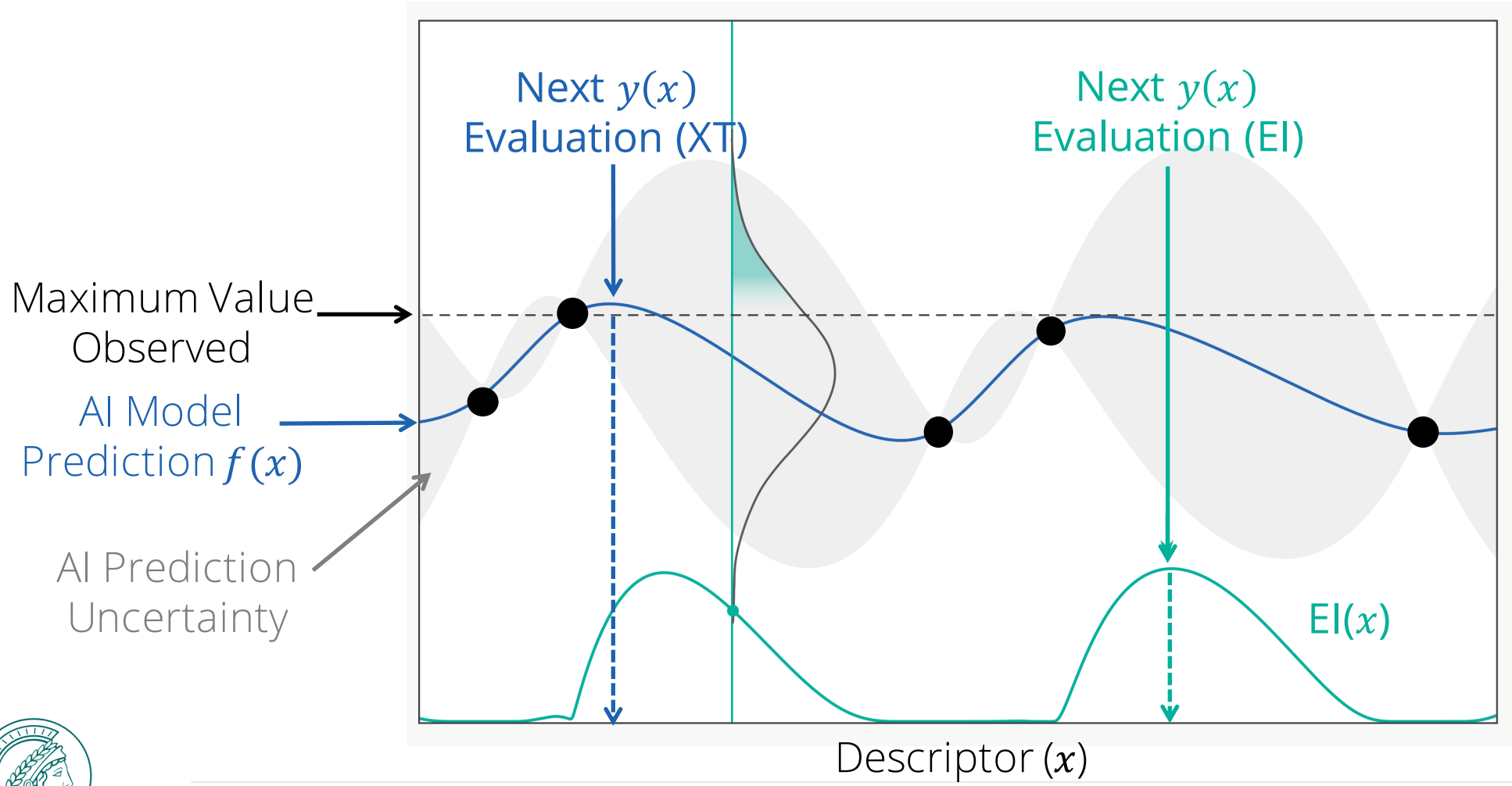
- Pure Exploitation (XT)



- XT Only Uses Predictions

Workflow 1: Identifying Perovskites with High Bulk Modulus

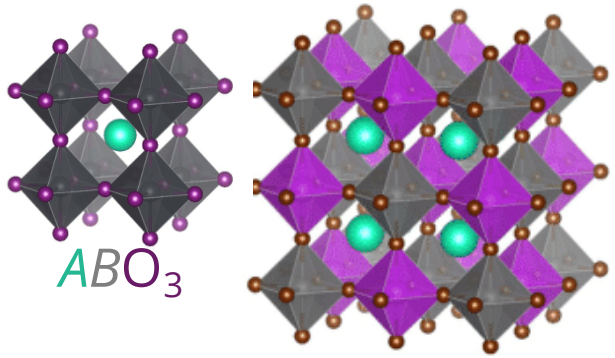
- **Reward:** Maximum B_0 Observed So Far
  - Pure Exploitation (XT)
  - Expected Improvement (EI)



- XT Only Uses Predictions
- EI Uses Predictions and Uncertainties
- EI Balances Model Exploitation and Exploration of Materials Space

Workflow 1: Identifying Perovskites with High Bulk Modulus

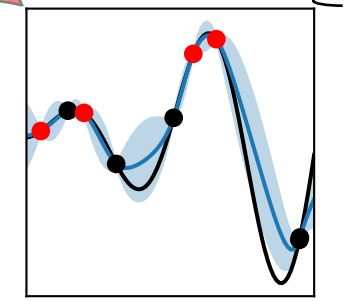
- Target Property (y):
  Bulk Modulus (B_0)



Initial Dataset (**814**)

0	y_0
...	...
n	y_n
$n+1$	y_{n+1}
$n+2$	y_{n+2}
$n+3$	y_{n+3}
$n+4$	y_{n+4}

AI Models
- Gaussian Processes (GP)
- Random Forests (RF)



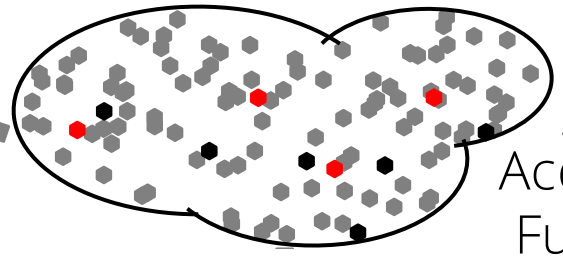
Descriptor (x)

Four Methods
- GP-XT
- GP-EI
- RF-XT
- RF-EI

Augment

Rank

Materials Space (**30 k**)



Acquisition Functions
- Pure Exploitation (XT)
- Expected Improvement (EI)

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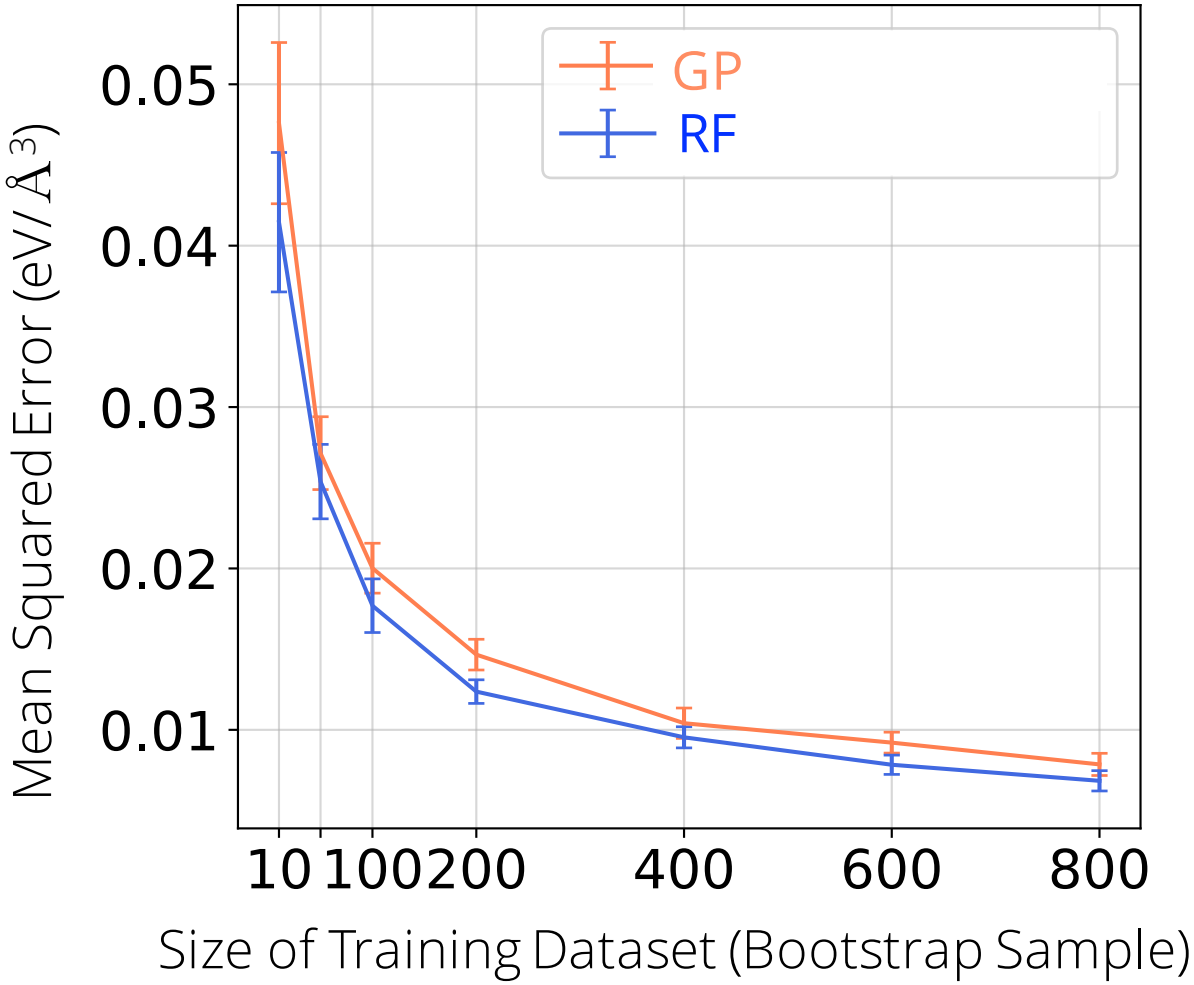
Workflow 1: Identifying Perovskites with High Bulk Modulus



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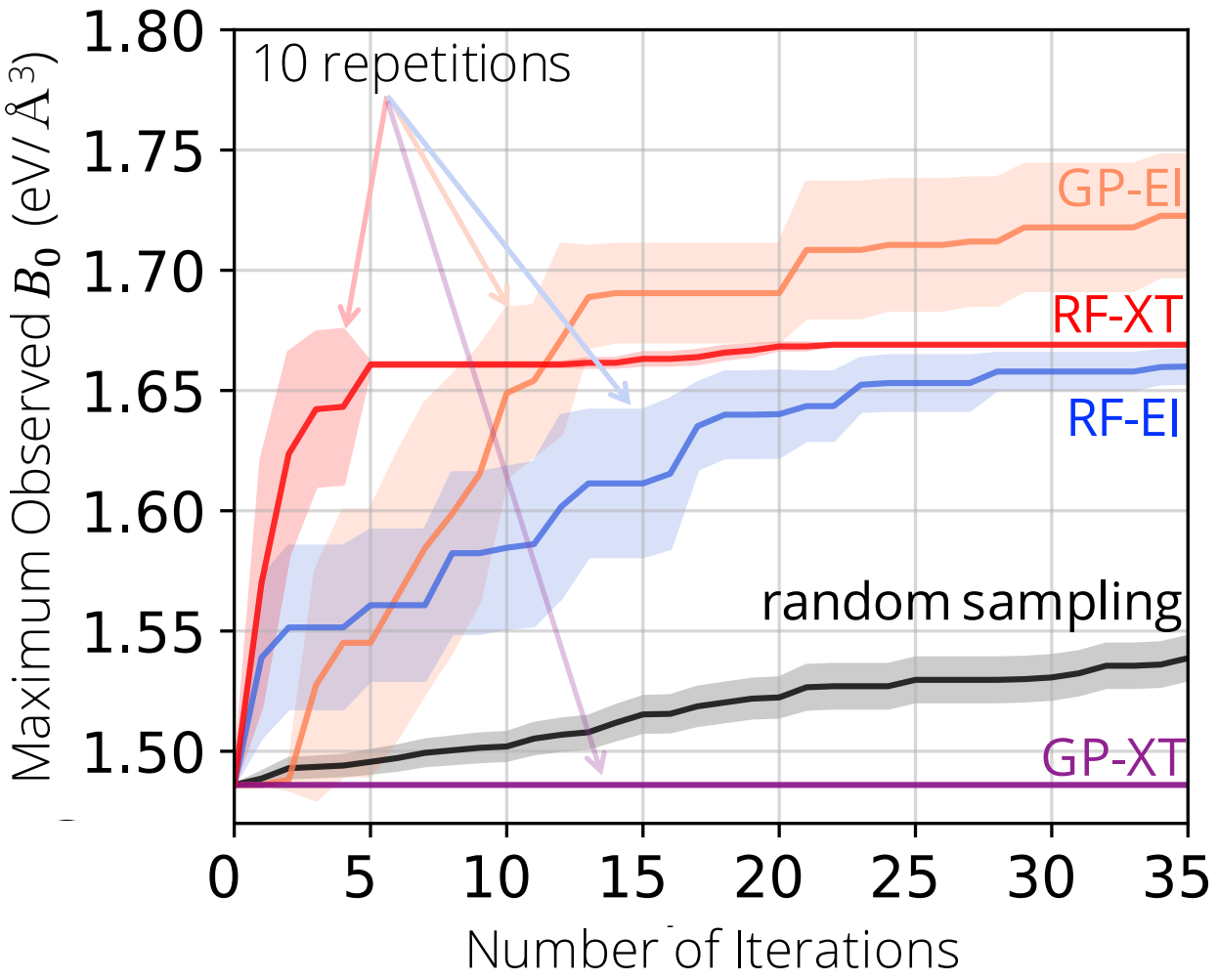
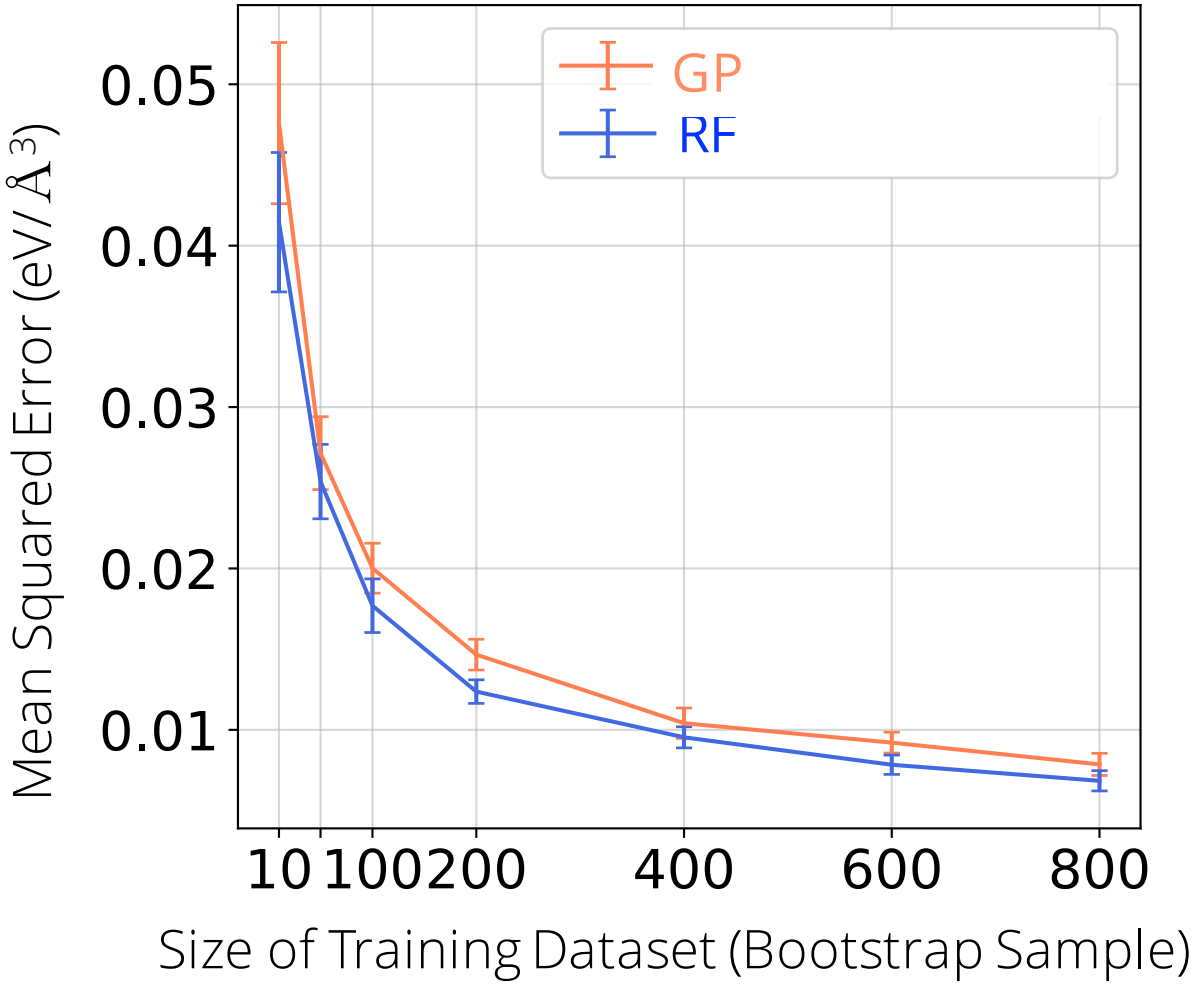
Workflow 1: Identifying Perovskites with High Bulk Modulus





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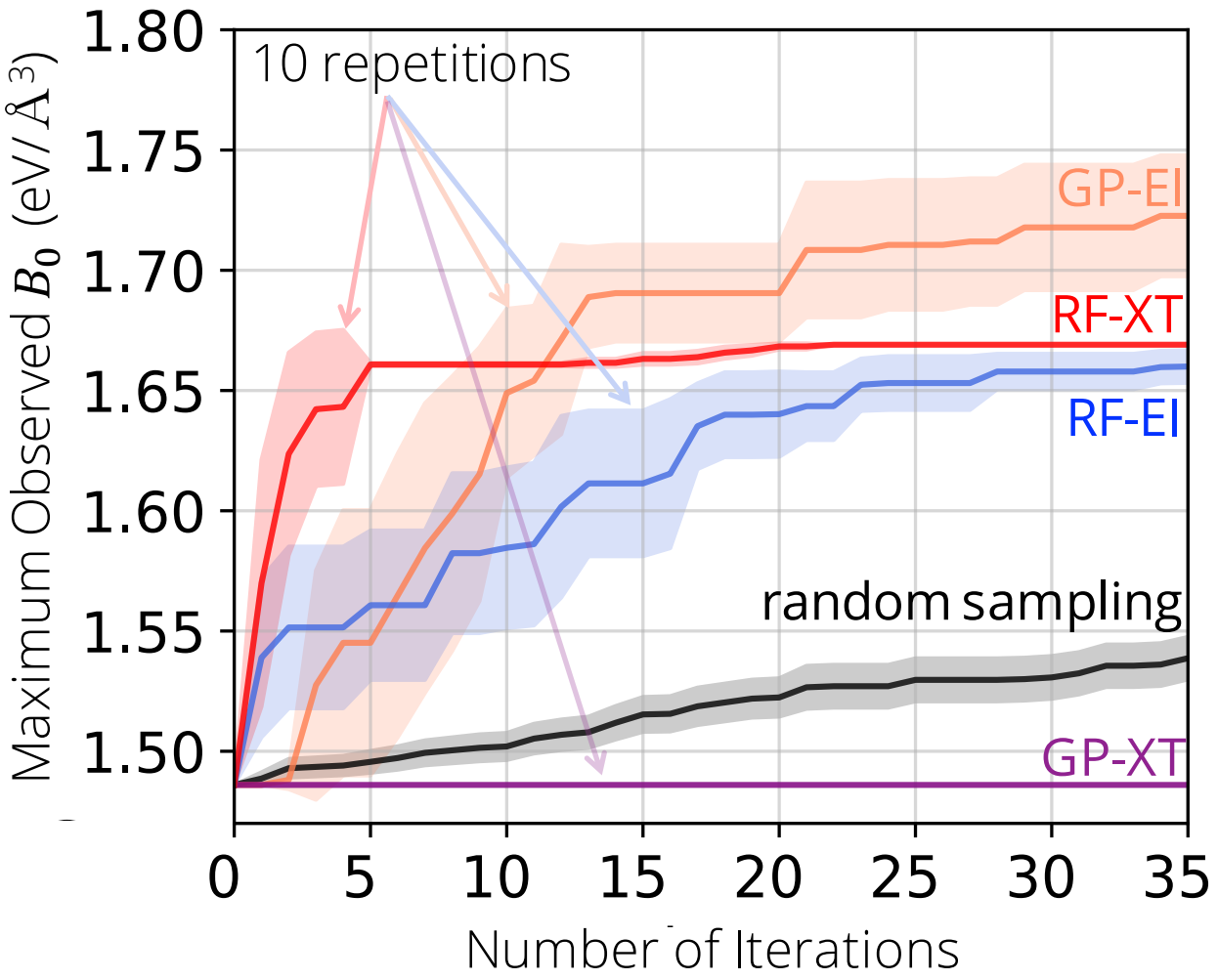
Workflow 1: Identifying Perovskites with High Bulk Modulus



- Efficiency of AI-Guided Workflow Depends On the Combination of AI Model and Acquisition Function
- Exploration (e.g., Guided By Uncertainty Estimates) Might Be Crucial
- Importance of Reliable Uncertainty Quantification (Overconfidence Issue)

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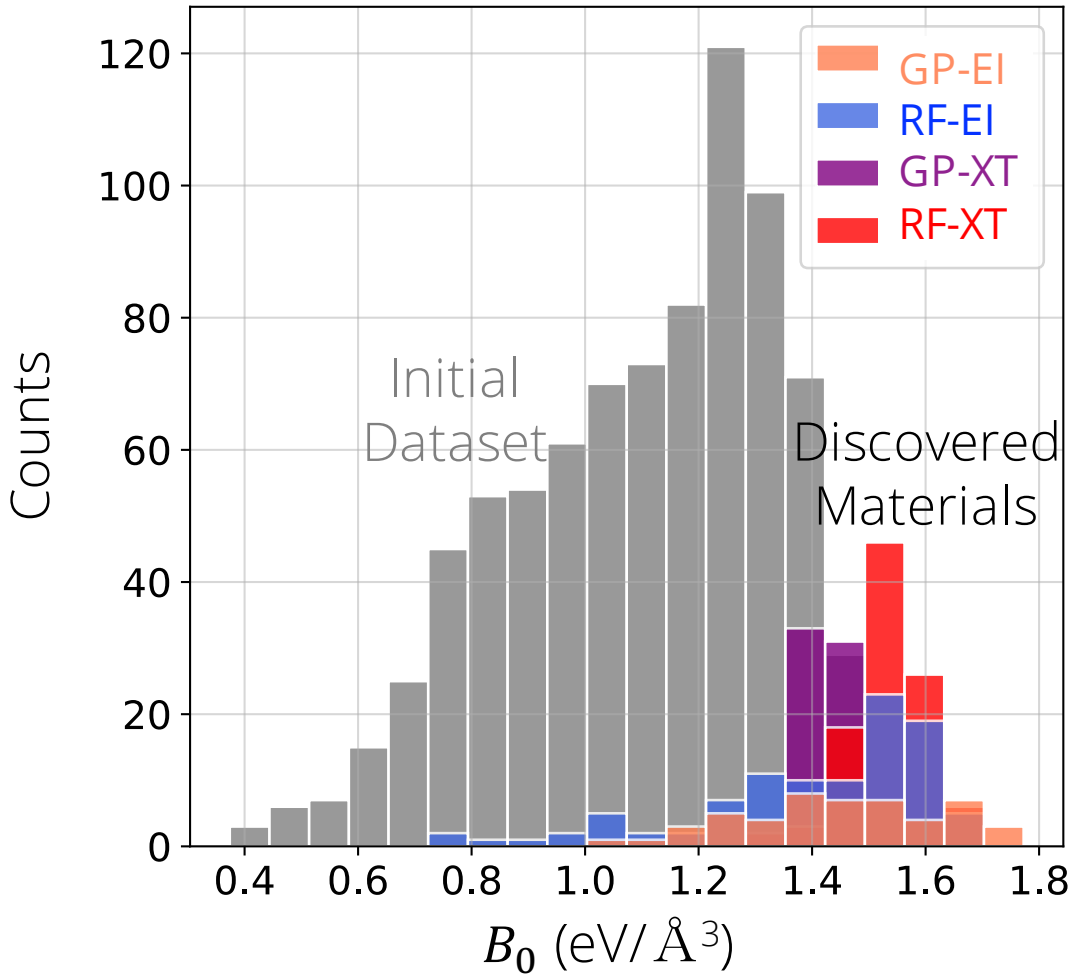
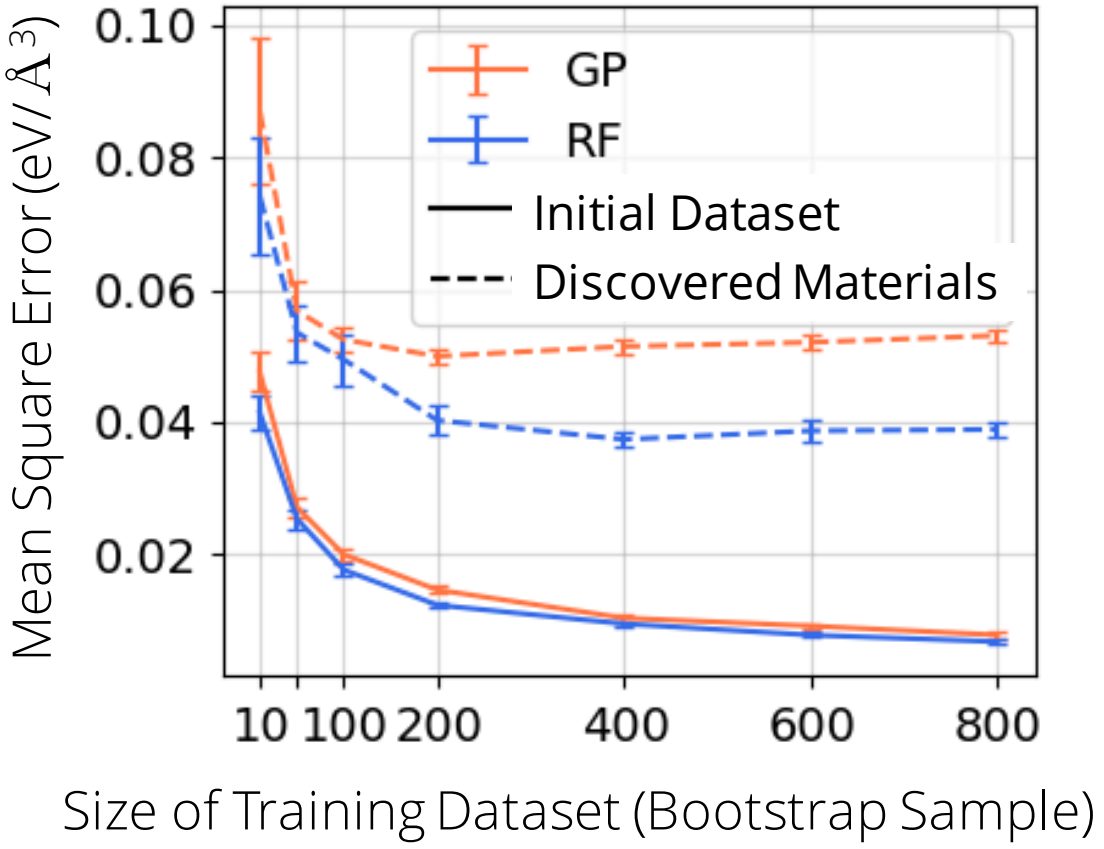
Workflow 1: Identifying Perovskites with High Bulk Modulus





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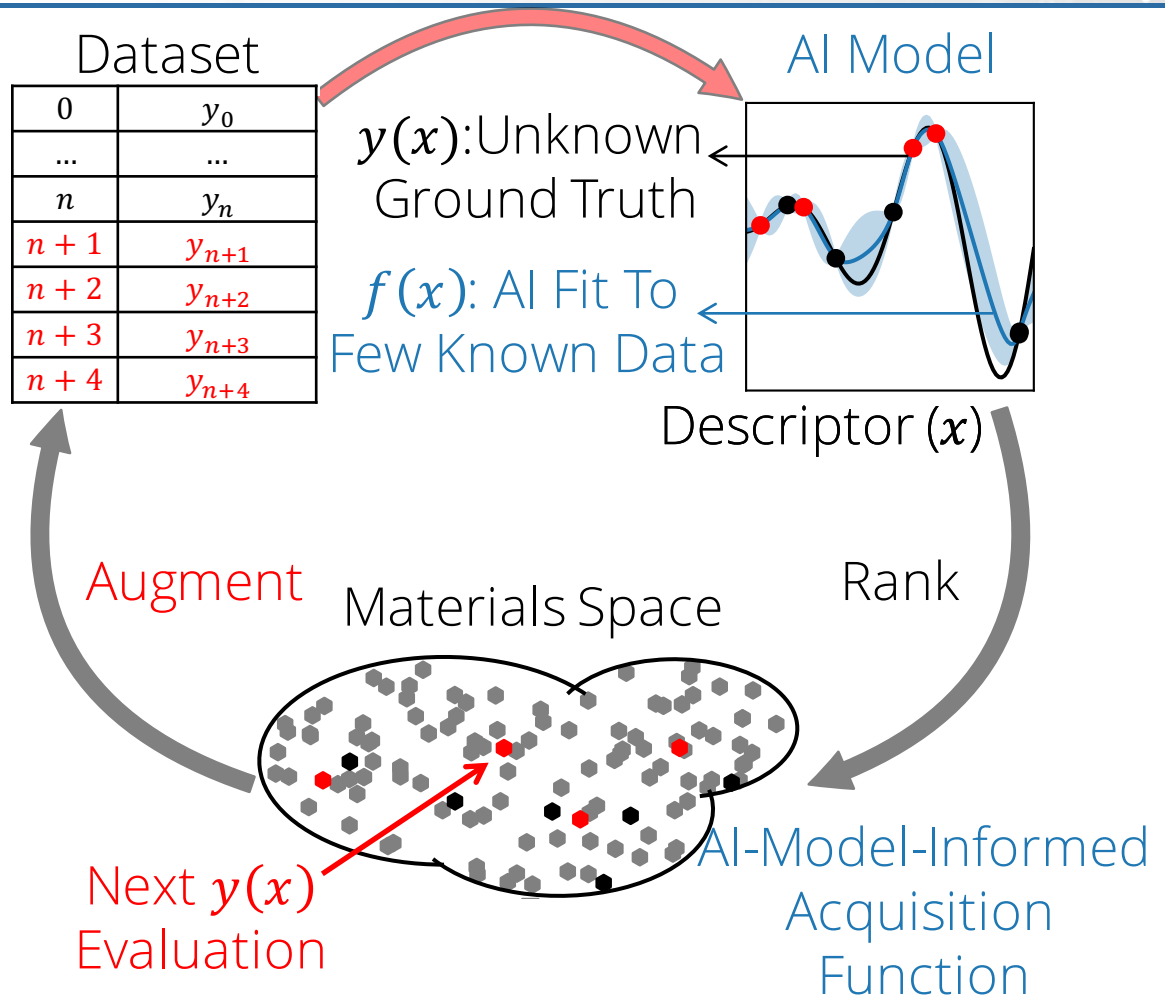
From Prediction to Action: AI-Guided Workflows for the Discovery of Materials with Optimal Properties

- Iterative Modelling and Data Acquisition Approach to Identify Materials with Desired Property Values (e.g., High)

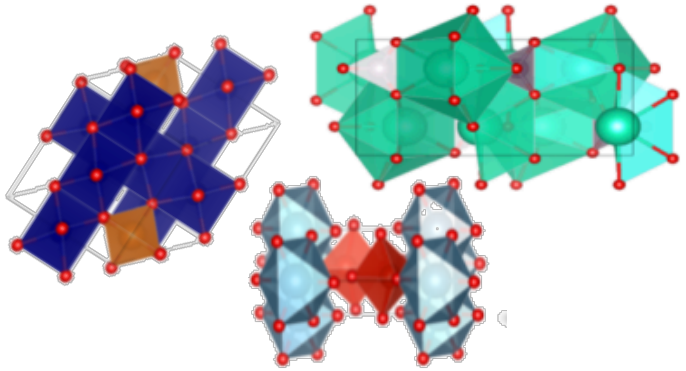
1. Impact of Choices of AI Model and Acquisition Function?

2. SISSO-Guided Workflow?



Workflow 2: Identifying Acid-Stable Oxides for Water Splitting

- **Target Property** (y): Decomposition Energy at OER Conditions pH=0, U=1.23 V ($\Delta G_{\mathbf{Pbx}}^{\mathbf{OER}}$)



Binary and Ternary Oxides

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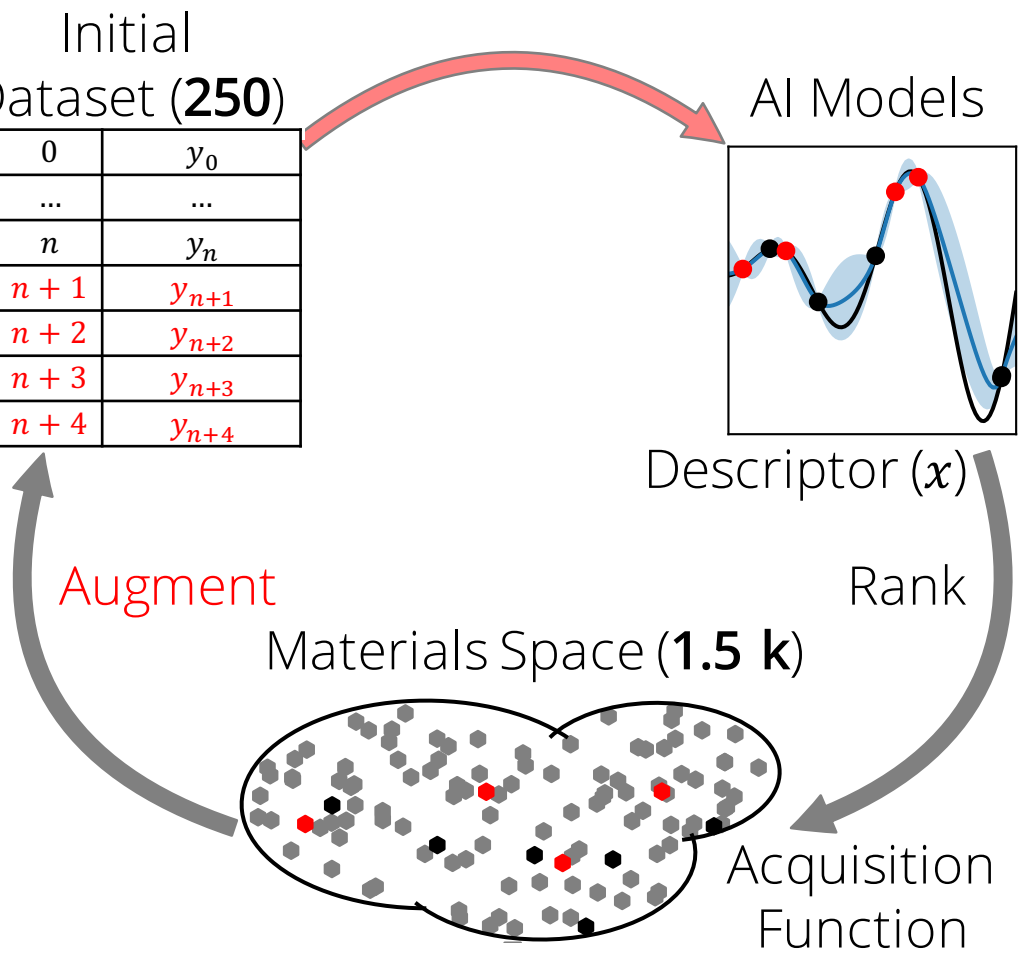

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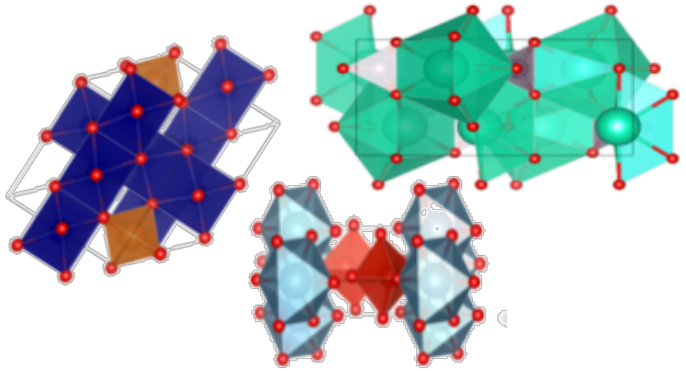
Workflow 2: Identifying Acid-Stable Oxides for Water Splitting

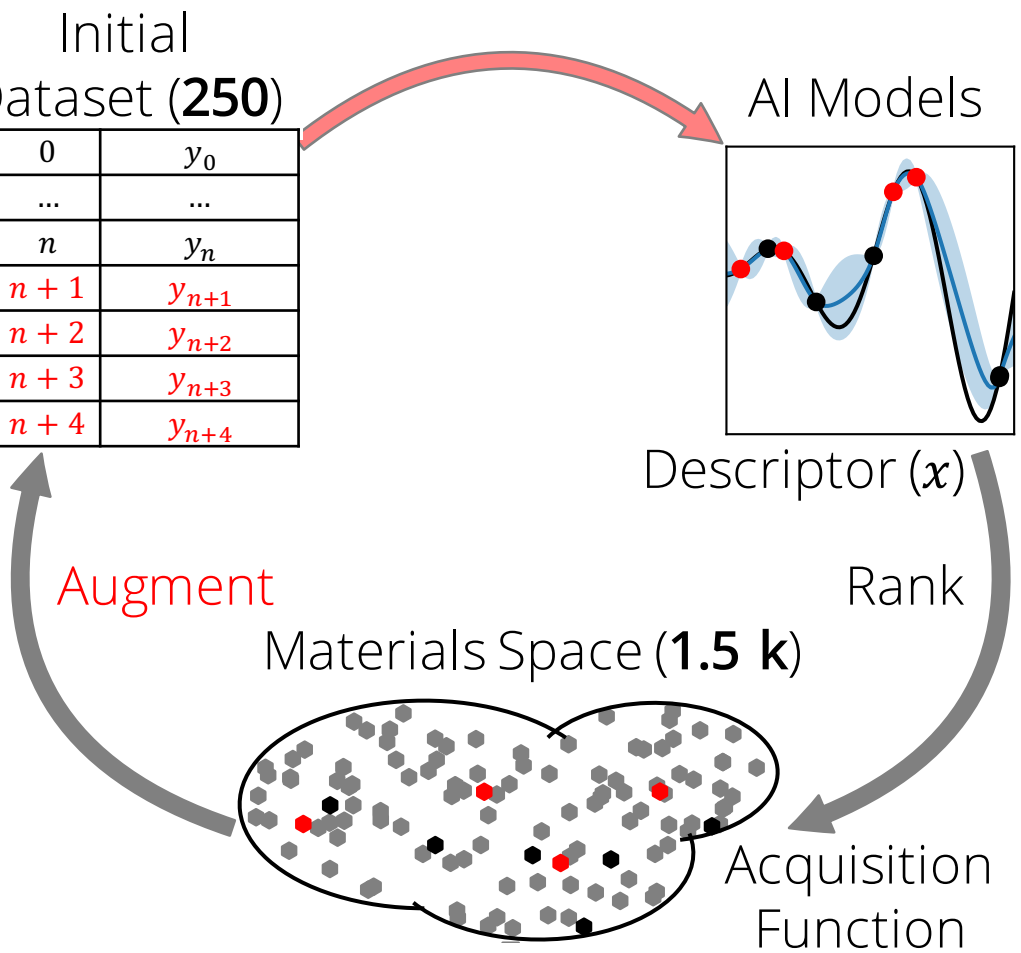
- **Target Property** (y): Decomposition Energy at OER Conditions pH=0, U=1.23 V ($\Delta G_{\mathbf{Pbx}}^{\mathbf{OER}}$)



Binary and Ternary Oxides

FHI-aims DFT-HSE06

The ab initio materials simulation package



- SISSO Approach
- Primary Features: 14 Physical Descriptive Parameters Depending on the Composition (e.g. Atomic Radii, Oxidation States)

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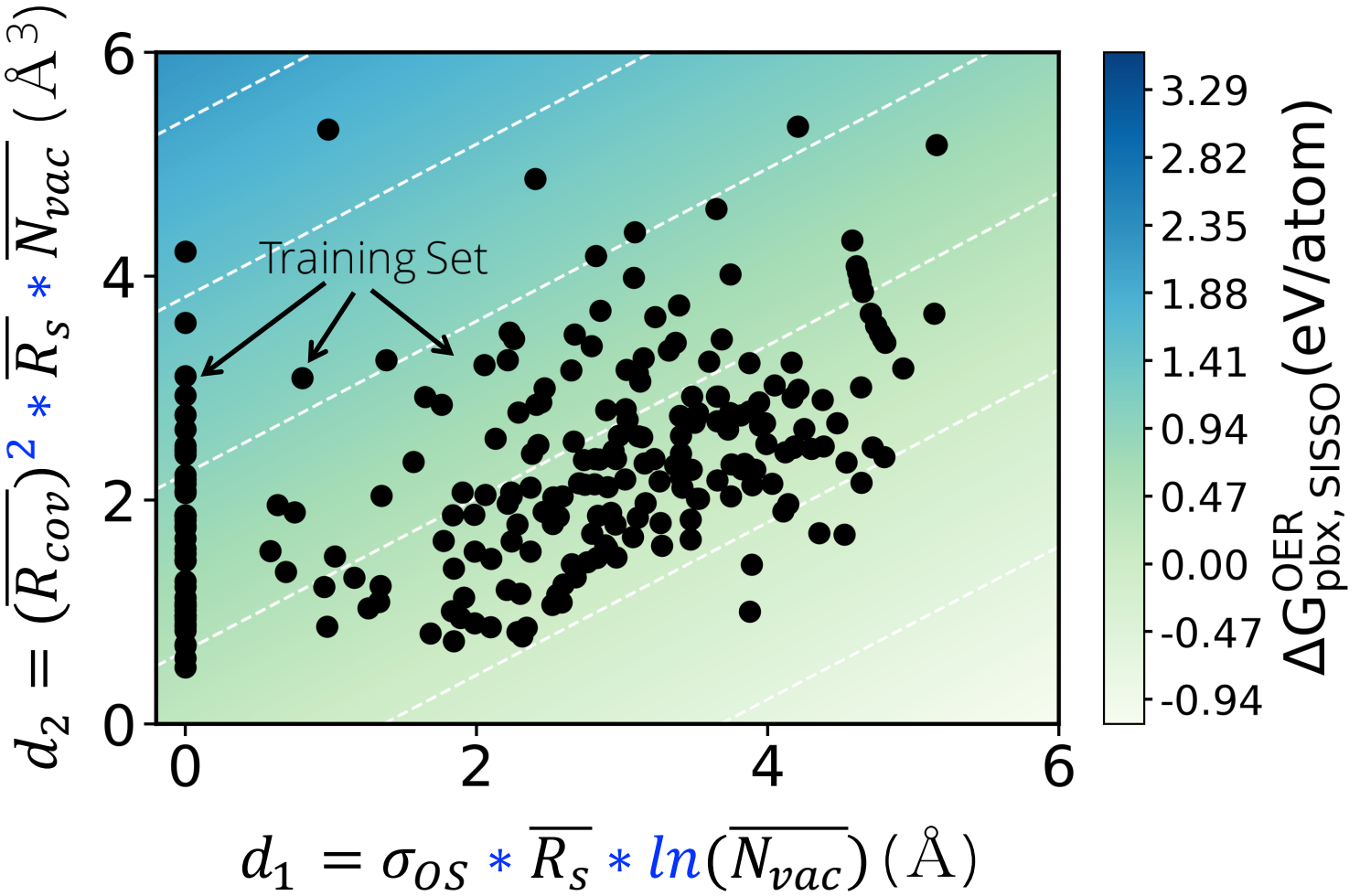
Workflow 2: Identifying Acid-Stable Oxides for Water Splitting



Key Parameters in the Descriptor

- σ_{OS}: Std. Dev. of Oxidation States
- $\overline{R_s}$: *s* Orbital Radius
- $\overline{N_{vac}}$: Number of Vacant Orbitals
- $\overline{R_{cov}}$: Covalent Radius

Average Across Cations

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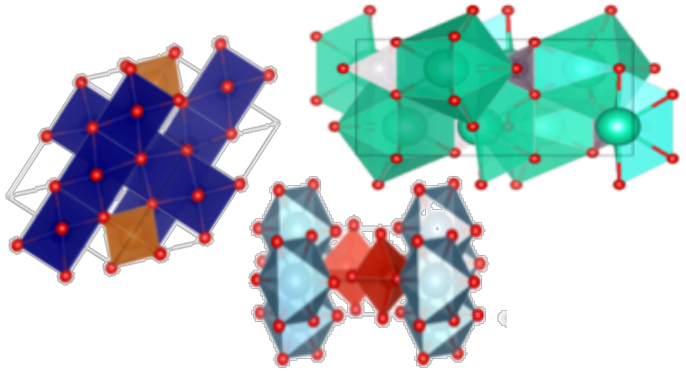
Workflow 2: Identifying Acid-Stable Oxides for Water Splitting

- **Target Property** (y): Decomposition Energy at OER Conditions pH=0, U=1.23 V ($\Delta G_{\mathrm{Pbx}}^{\mathrm{OER}}$)



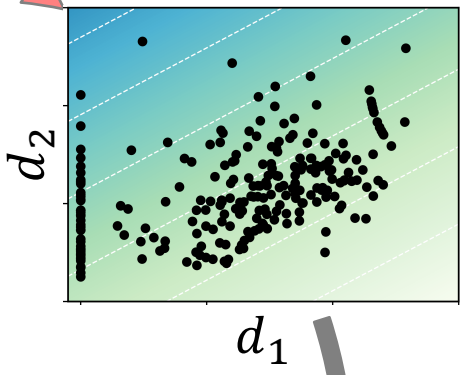
Binary and Ternary Oxides

FHI-aims DFT-HSE06
The ab initio materials simulation package

Initial Dataset (**250**)

0	y_0
...	...
n	y_n
$n+1$	y_{n+1}
$n+2$	y_{n+2}
$n+3$	y_{n+3}
$n+4$	y_{n+4}

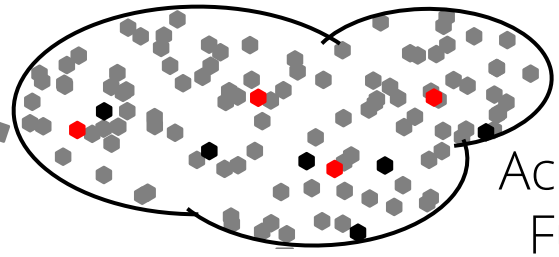
AI Models



Augment

Rank

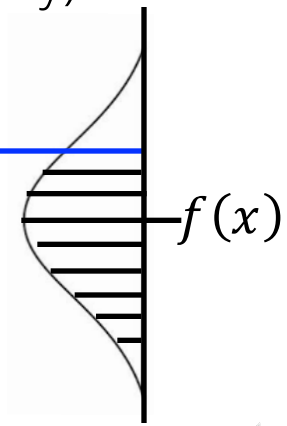
Materials Space (**1.5 k**)



Acquisition Function

- SISSO Approach
  - **Reward:** No. of Stable Materials
  - Probability of Feasibility POF (Prediction and Uncertainty)

$\Delta G_{\mathrm{Pbx}}^{\mathrm{OER}} < 0.10$ eV/atom



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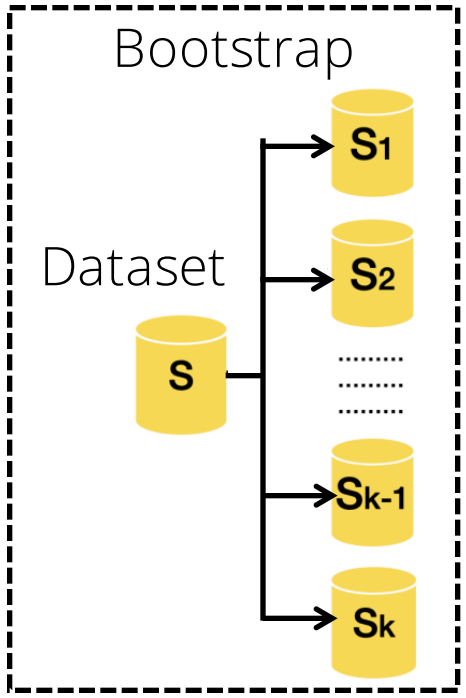
Workflow 2: Identifying Acid-Stable Oxides for Water Splitting

Creating Ensembles of SISSO Models: 1. (Standard) Bagging



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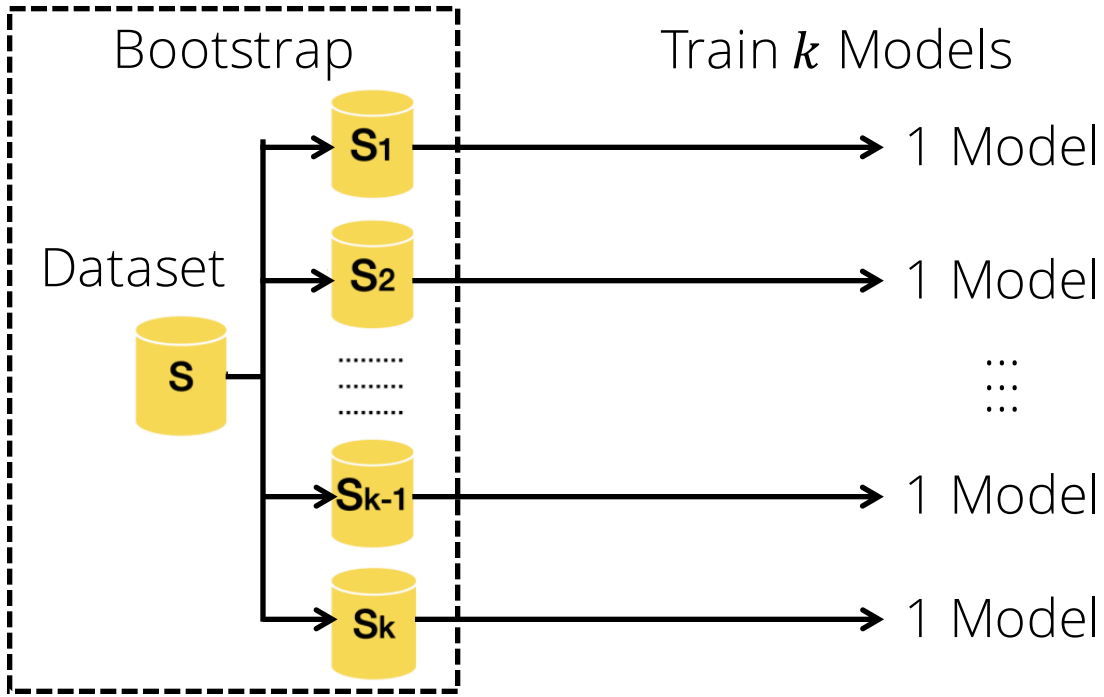
Workflow 2: Identifying Acid-Stable Oxides for Water Splitting

Creating Ensembles of SISSO Models: 1. (Standard) Bagging



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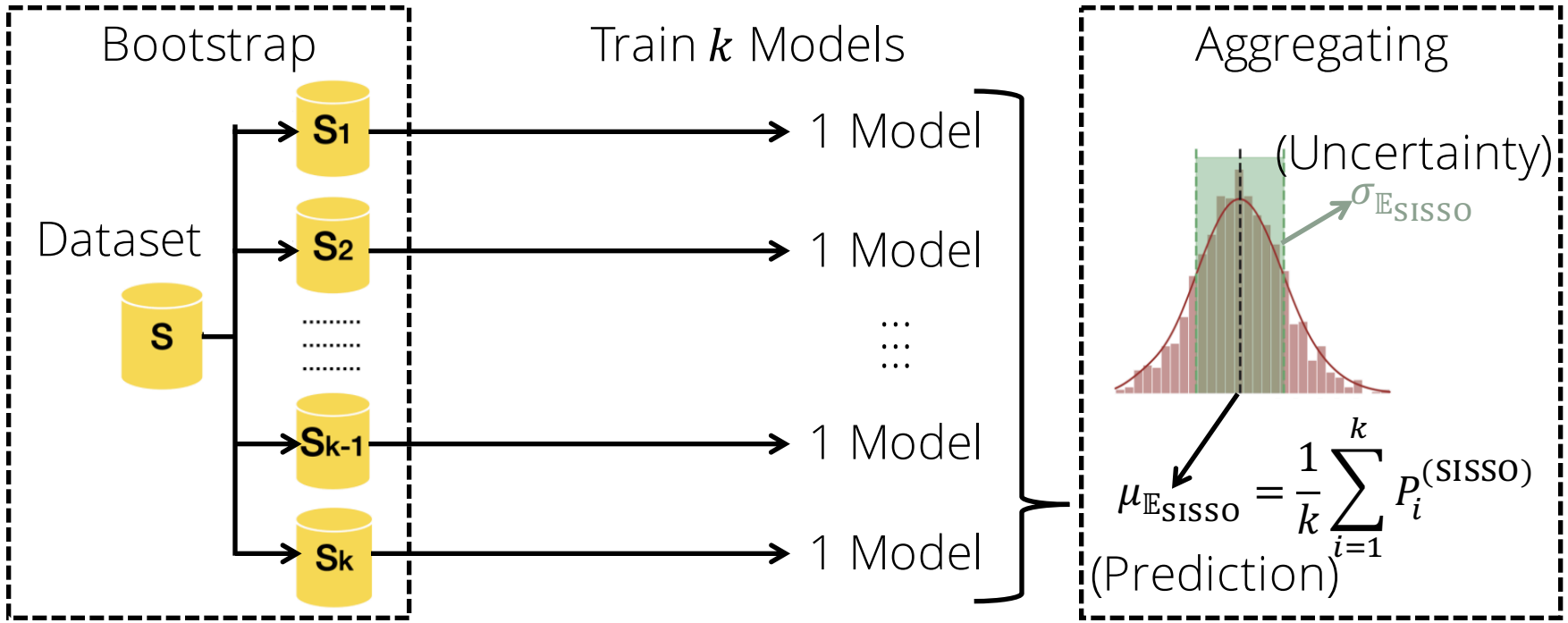
Workflow 2: Identifying Acid-Stable Oxides for Water Splitting

Creating Ensembles of SISSO Models: 1. (Standard) Bagging



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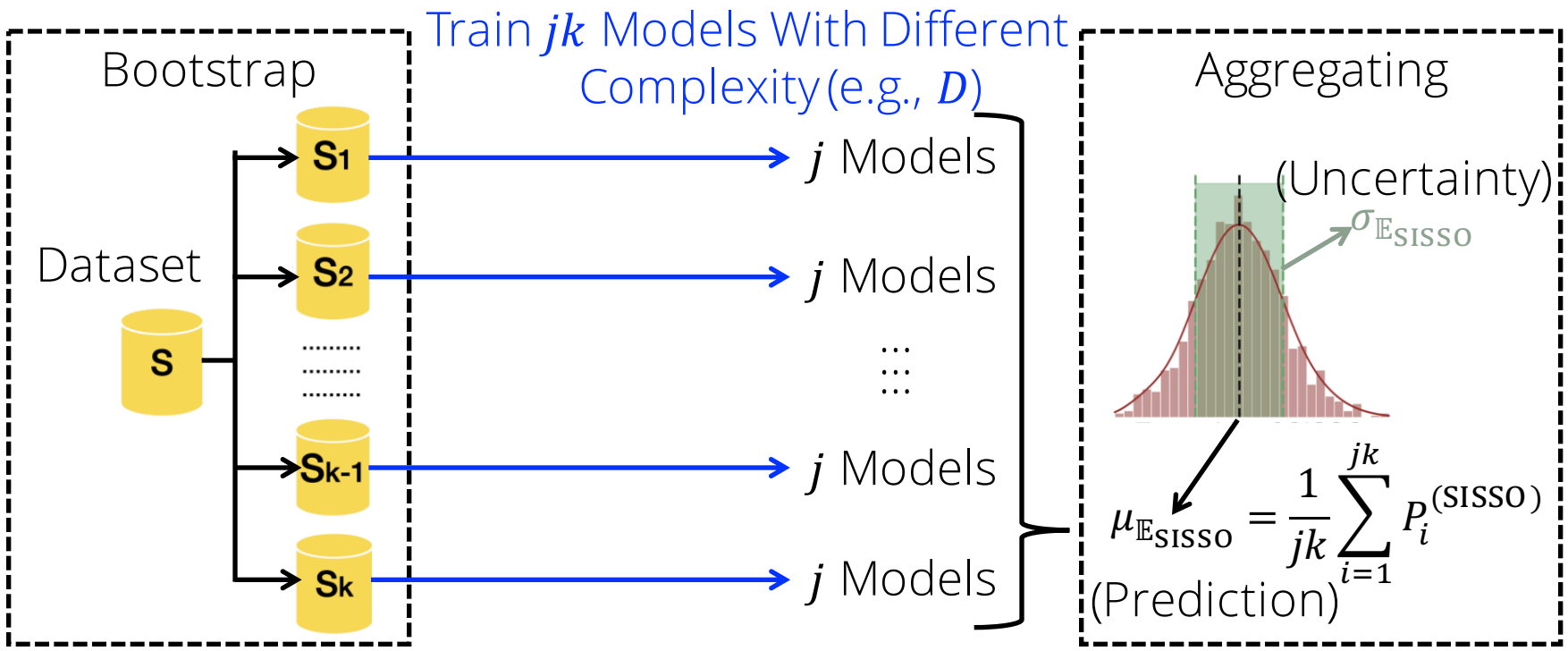
Workflow 2: Identifying Acid-Stable Oxides for Water Splitting

Creating Ensembles of SISSO Models: 2. Bagging with Multiple Model Complexities



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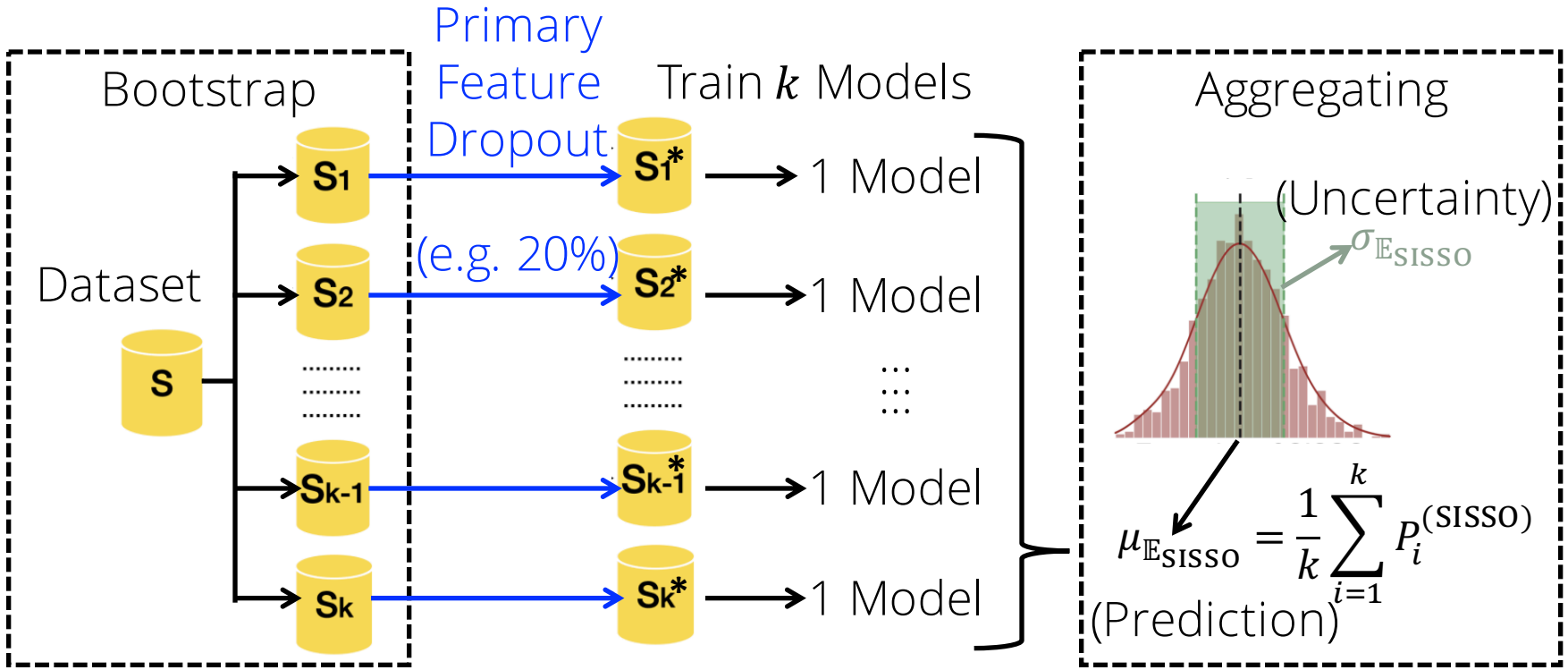
Workflow 2: Identifying Acid-Stable Oxides for Water Splitting

Creating Ensembles of SISSO Models: 3. Bagging with Monte-Carlo Dropout of Primary Features



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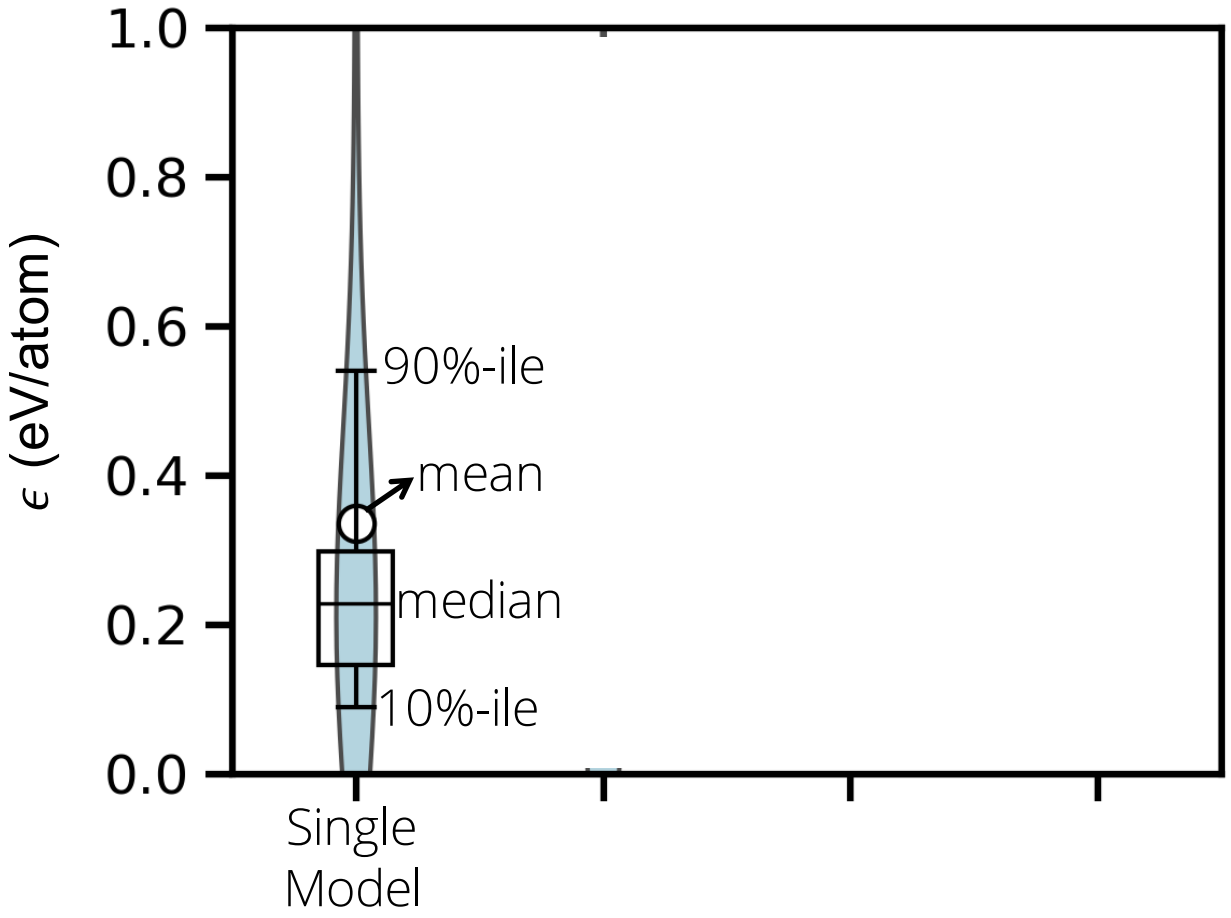
Workflow 2: Identifying Acid-Stable Oxides for Water Splitting

Assessing the Quality of Mean Predictions of SISSO-Model Ensembles

Absolute Prediction Error
(20% Left-Out Materials)

$$\epsilon = |\Delta G^{\mathrm{OER}}_{\mathrm{Pbx}} - \Delta G^{\mathrm{OER}}_{\mathrm{Pbx},\mathbb{E}_{\mathrm{SISSO}}}|$$



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Workflow 2: Identifying Acid-Stable Oxides for Water Splitting

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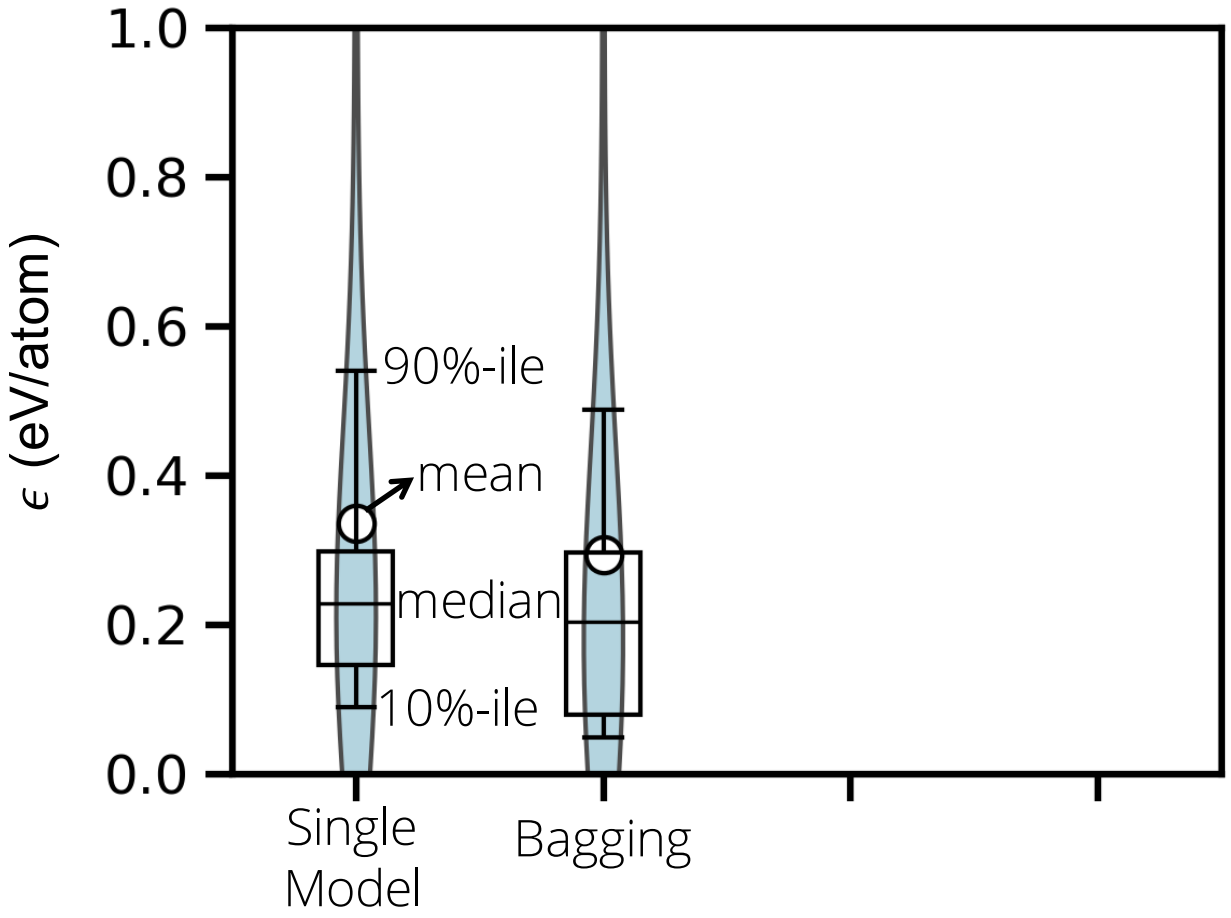

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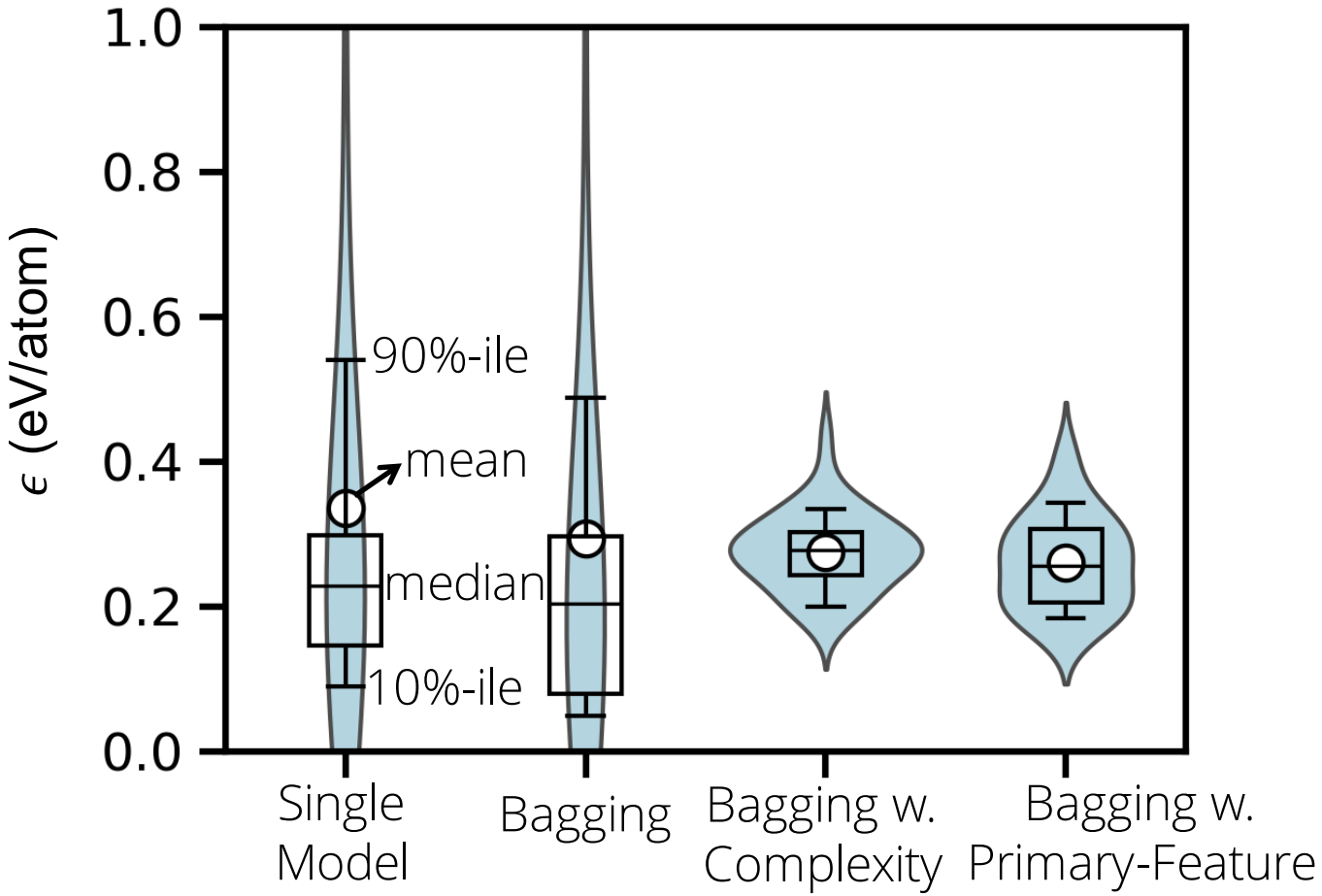
Workflow 2: Identifying Acid-Stable Oxides for Water Splitting

Assessing the Quality of Mean Predictions of SISSO-Model Ensembles

Absolute Prediction Error (20% Left-Out Materials)

$$\epsilon = |\Delta G^{\mathrm{OER}}_{\mathrm{Pbx}} - \Delta G^{\mathrm{OER}}_{\mathrm{Pbx},\mathbb{E}_{\mathrm{SISSO}}}|$$

- Proposed Ensemble Approaches Mitigate High Errors



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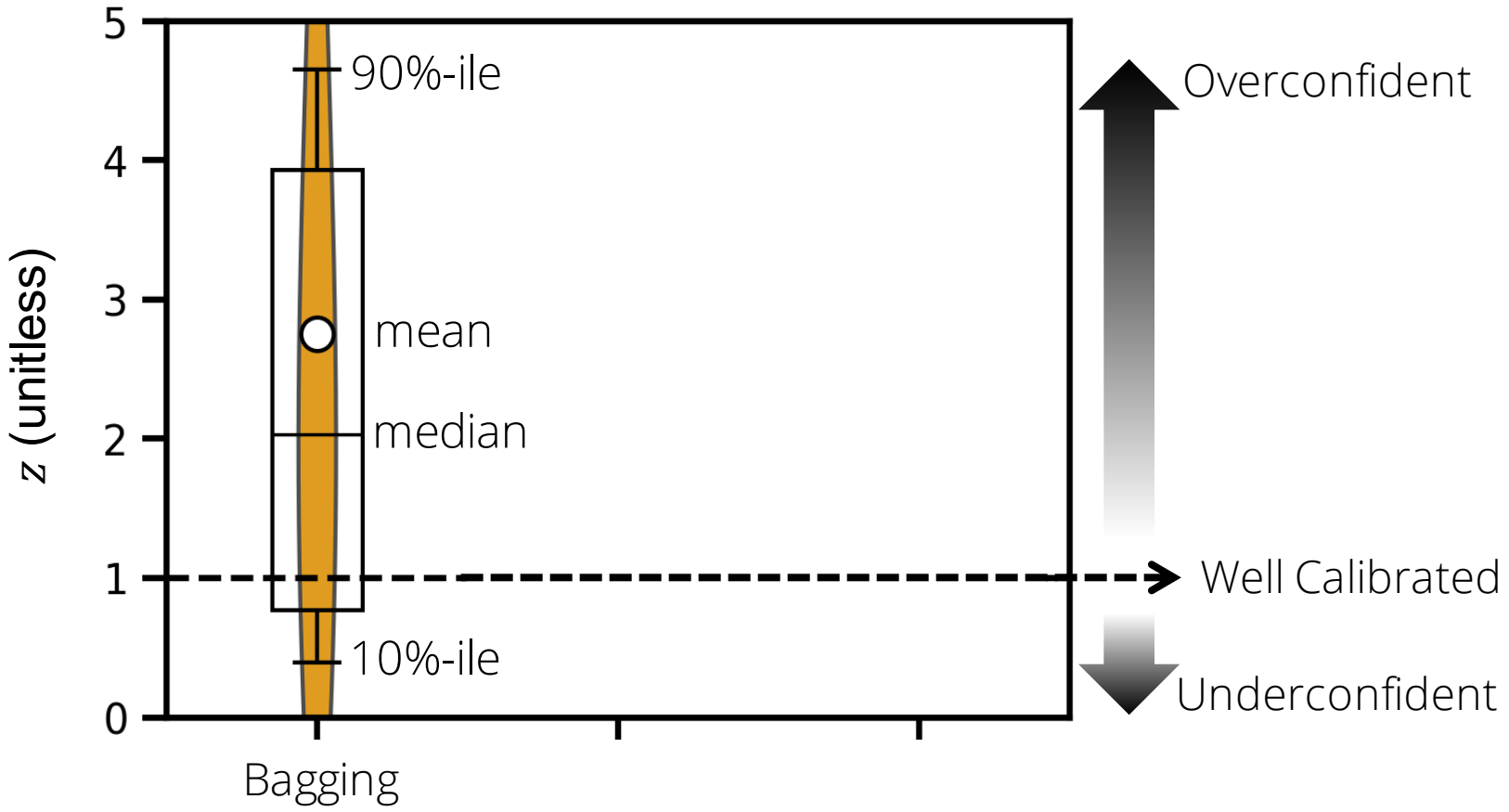
Workflow 2: Identifying Acid-Stable Oxides for Water Splitting

Assessing the Quality of Uncertainty Estimates of SISSO-Model Ensembles

Miscalibration Score
(20% Left-Out Materials)

$$z = \frac{|\Delta G^{\mathrm{OER}}_{\mathrm{Pbx}} - \Delta G^{\mathrm{OER}}_{\mathrm{Pbx},\mathbb{E}_{\mathrm{SISSO}}}|}{\sigma_{\mathbb{E}_{\mathrm{SISSO}}}}$$



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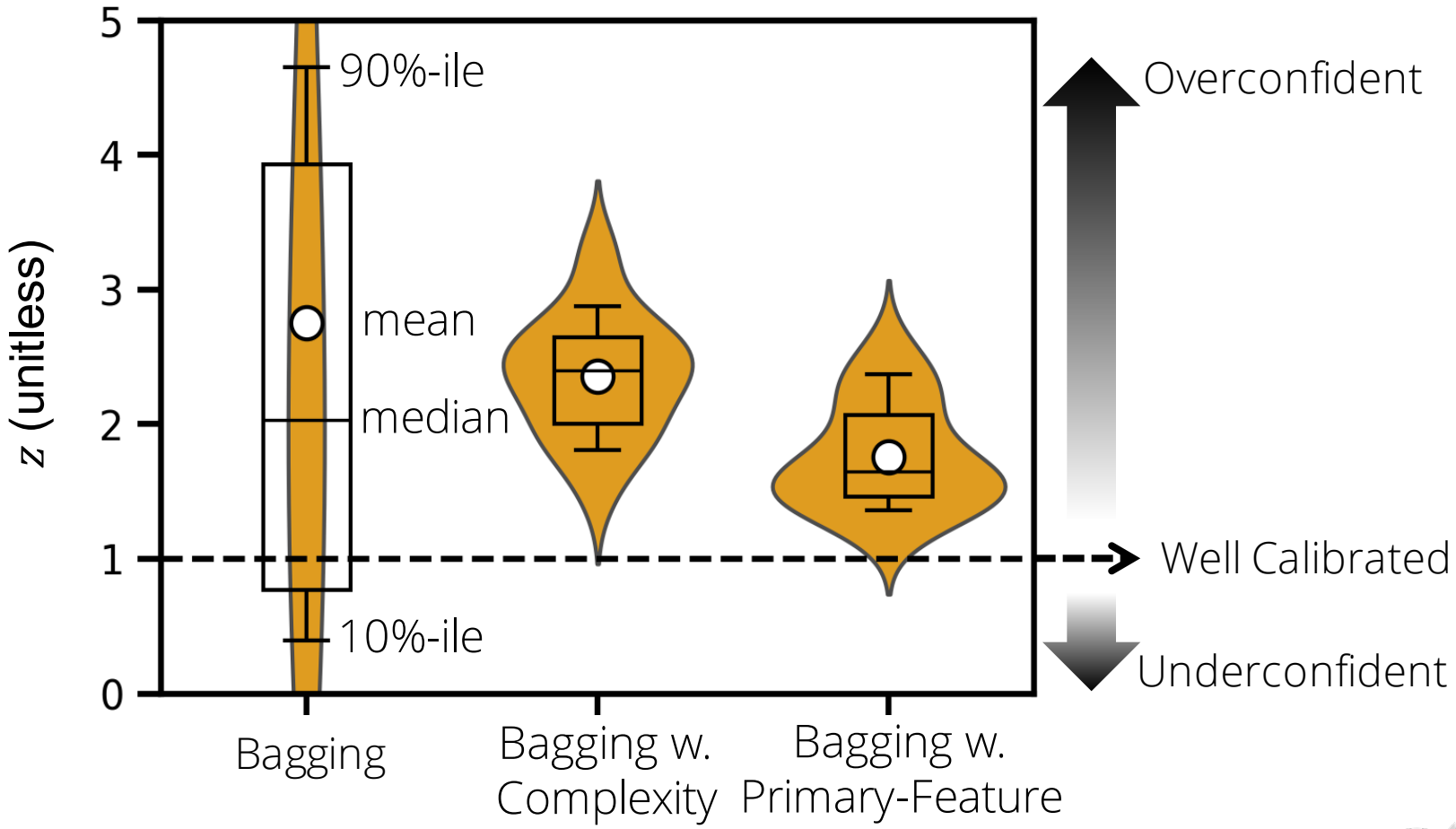
Workflow 2: Identifying Acid-Stable Oxides for Water Splitting

Assessing the Quality of Uncertainty Estimates of SISSO-Model Ensembles

Miscalibration Score
(20% Left-Out Materials)

$$z = \frac{|\Delta G^{\mathrm{OER}}_{\mathrm{Pbx}} - \Delta G^{\mathrm{OER}}_{\mathrm{Pbx},\mathbb{E}_{\mathrm{SISSO}}}|}{\sigma_{\mathbb{E}_{\mathrm{SISSO}}}}$$

- Use of Primary-Feature Dropout Mitigates Overconfidence Issue



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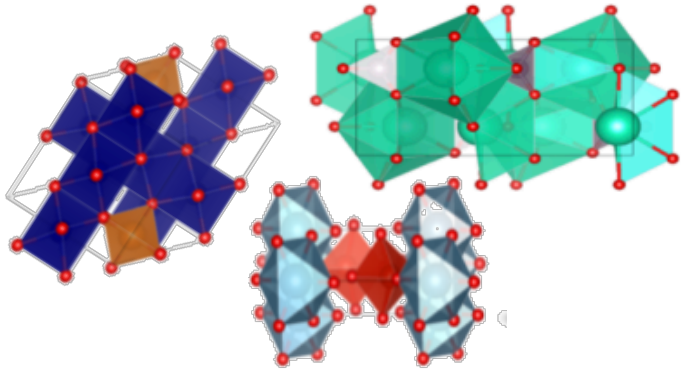
Workflow 2: Identifying Acid-Stable Oxides for Water Splitting

- **Target Property** (y): Decomposition Energy at OER Conditions pH=0, U=1.23 V ($\Delta G_{\mathrm{Pbx}}^{\mathrm{OER}}$)



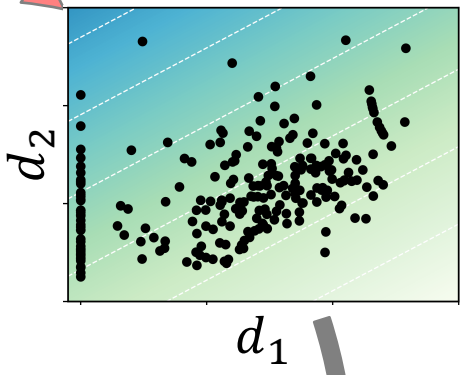
Binary and Ternary Oxides

FHI-aims The ab initio materials simulation package DFT-HSE06

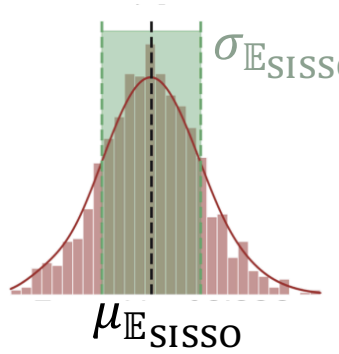
Initial Dataset (**250**)

0	y_0
...	...
n	y_n
$n+1$	y_{n+1}
$n+2$	y_{n+2}
$n+3$	y_{n+3}
$n+4$	y_{n+4}

AI Models

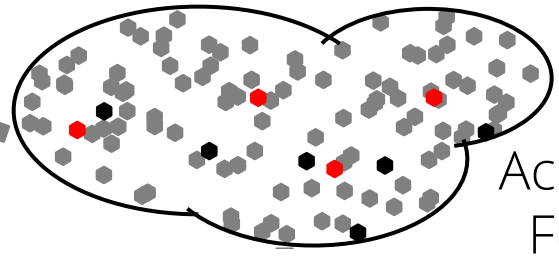


- SISSO Ensembles (Primary-Feature Dropout)



Rank

Materials Space (**1.5 k**)



Augment

Acquisition Function

- Probability of Feasibility

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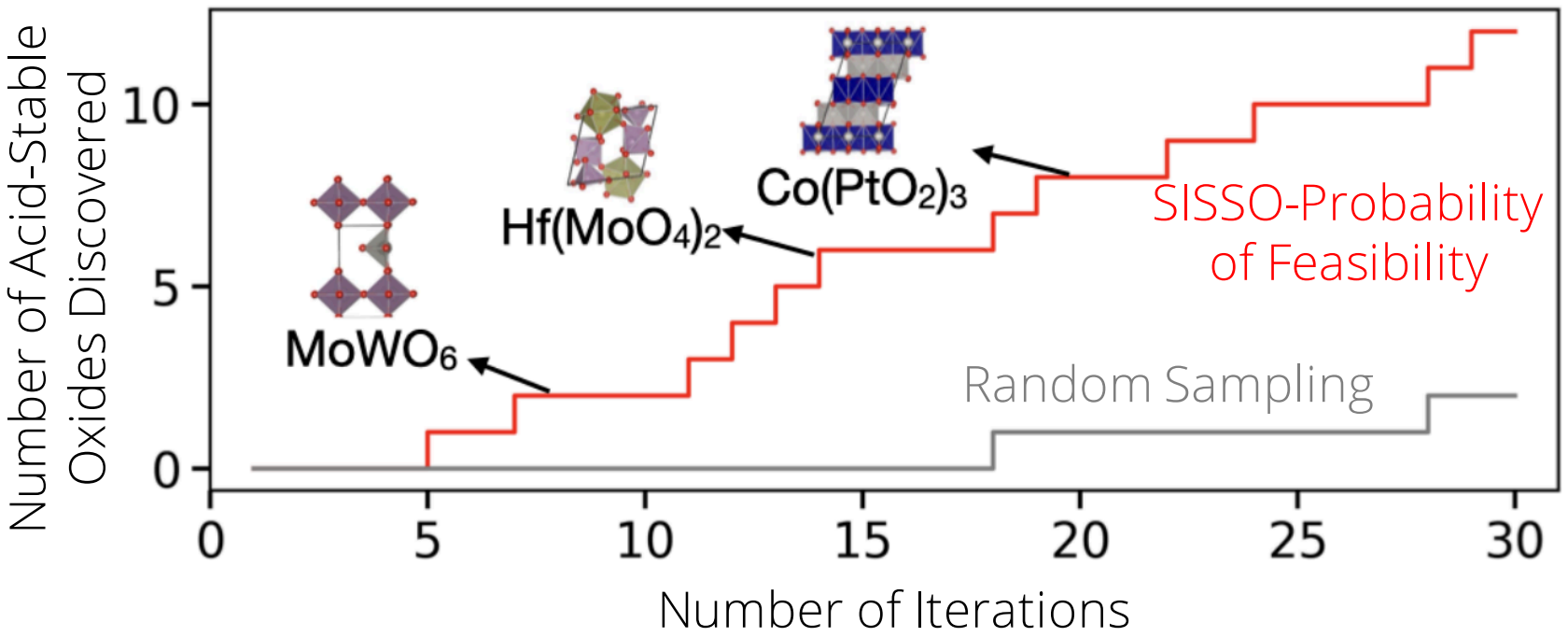
Workflow 2: Identifying Acid-Stable Oxides for Water Splitting



- Workflow Enabled the Discovery of 12 Stable Oxides, Out of 1.5 k Candidates in 30 Iterations

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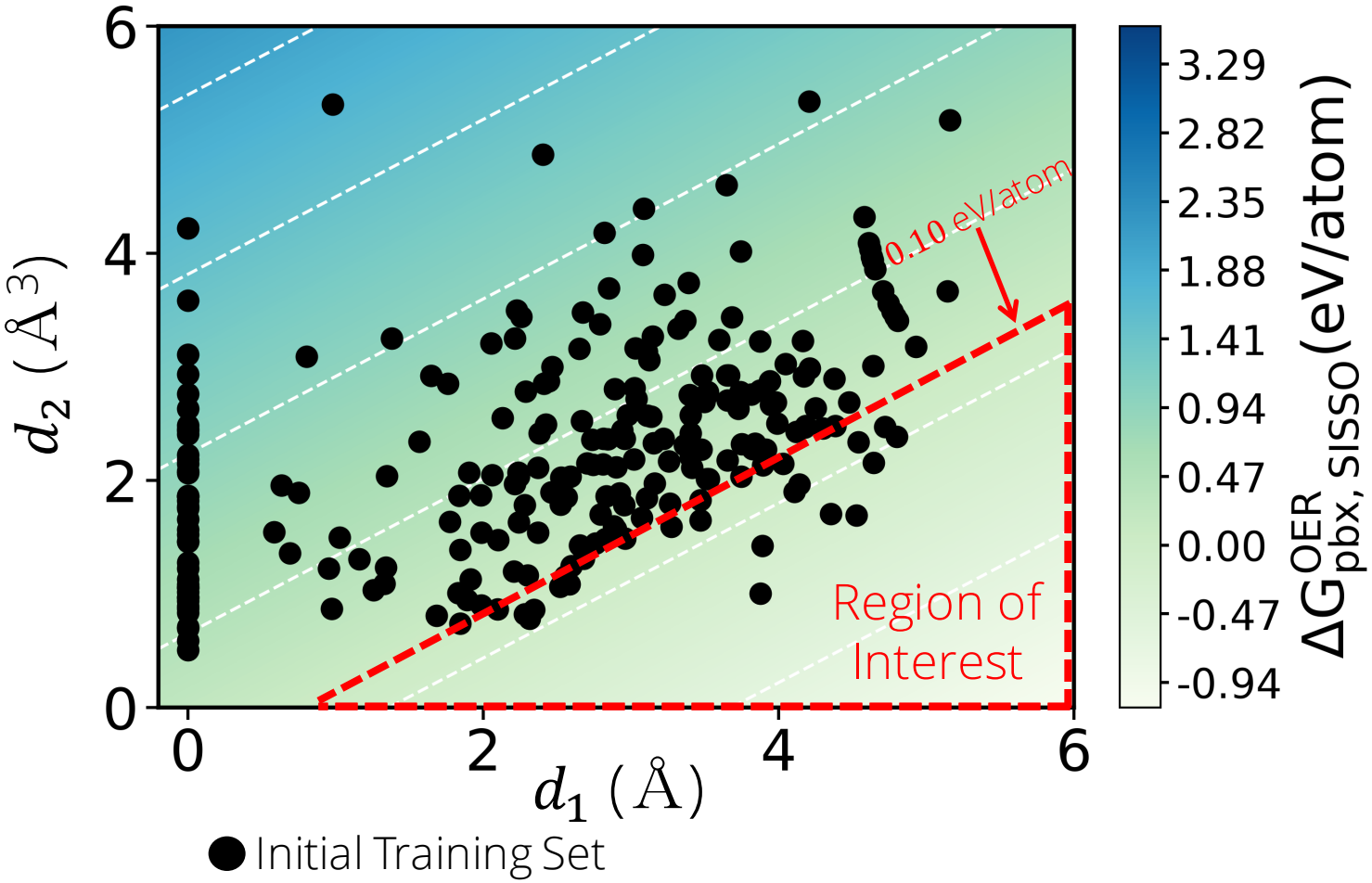
Workflow 2: Identifying Acid-Stable Oxides for Water Splitting



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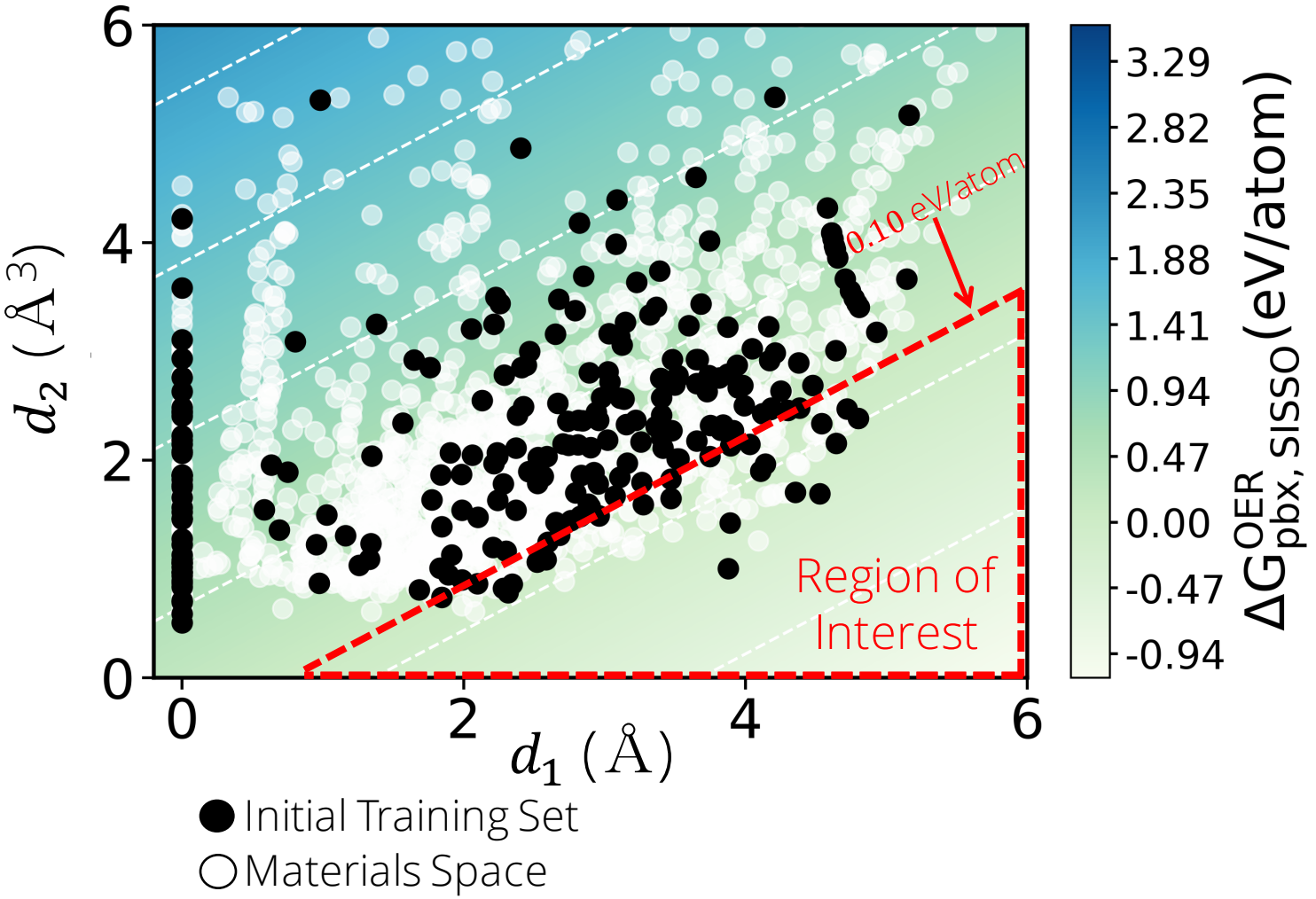
Workflow 2: Identifying Acid-Stable Oxides for Water Splitting



- Only Few Materials Stable

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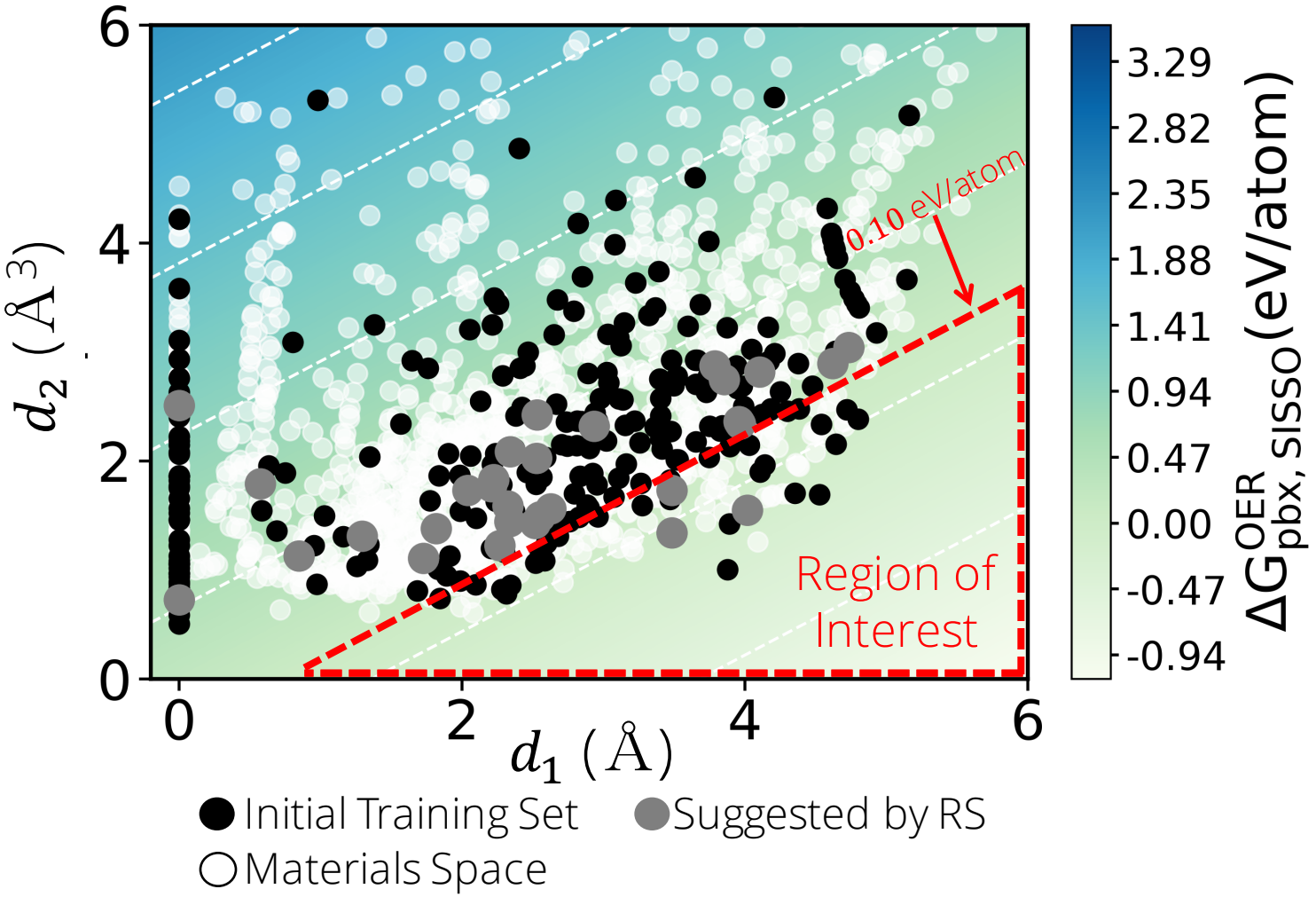
Workflow 2: Identifying Acid-Stable Oxides for Water Splitting



- Only Few Materials Stable

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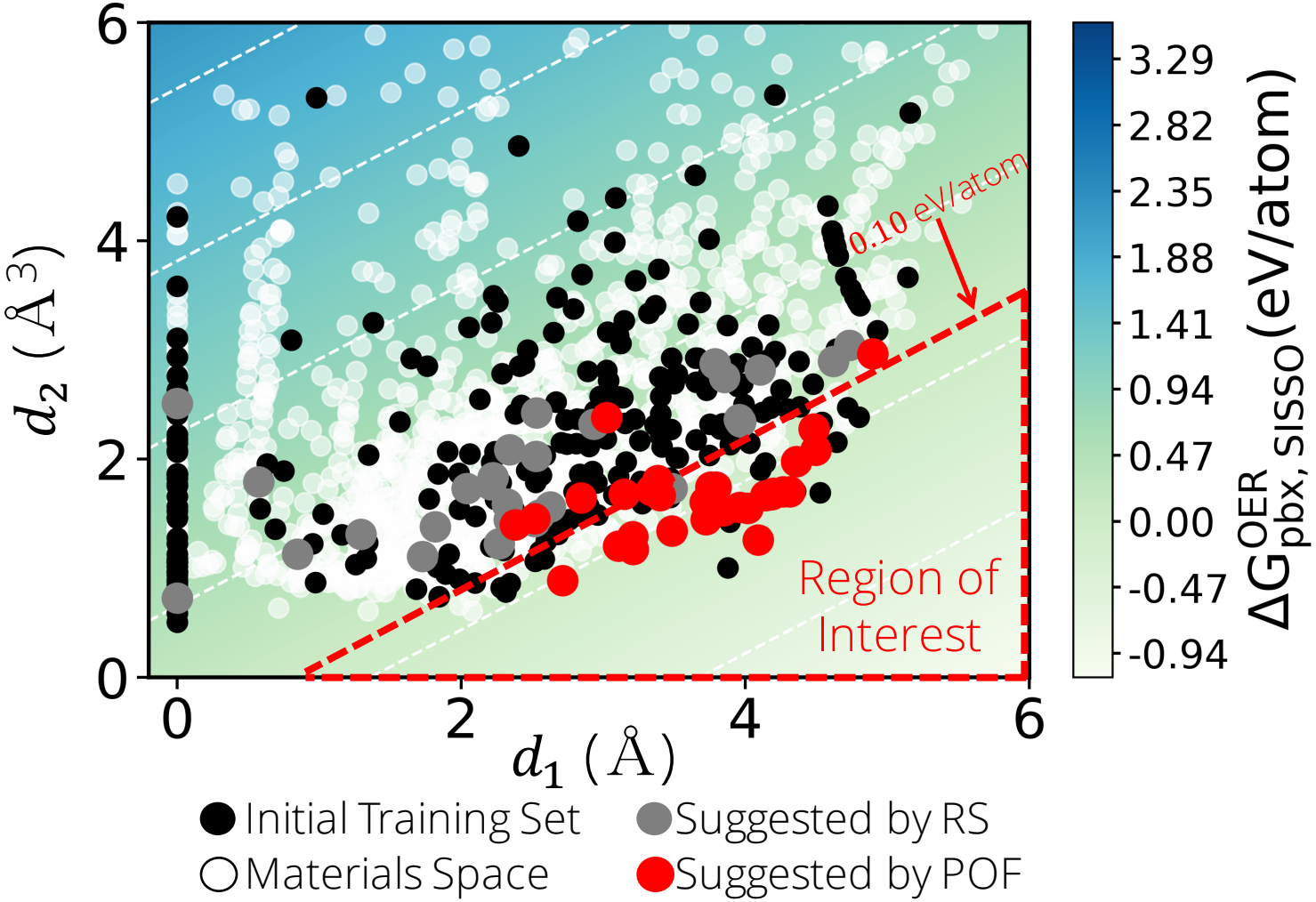
Workflow 2: Identifying Acid-Stable Oxides for Water Splitting



- Only Few Materials Stable
- Most Stable Materials Correctly Predicted by Initial SISSO Model
- Some Stable Oxides Identified by Workflow Incorrectly Predicted Unstable By Initial Model

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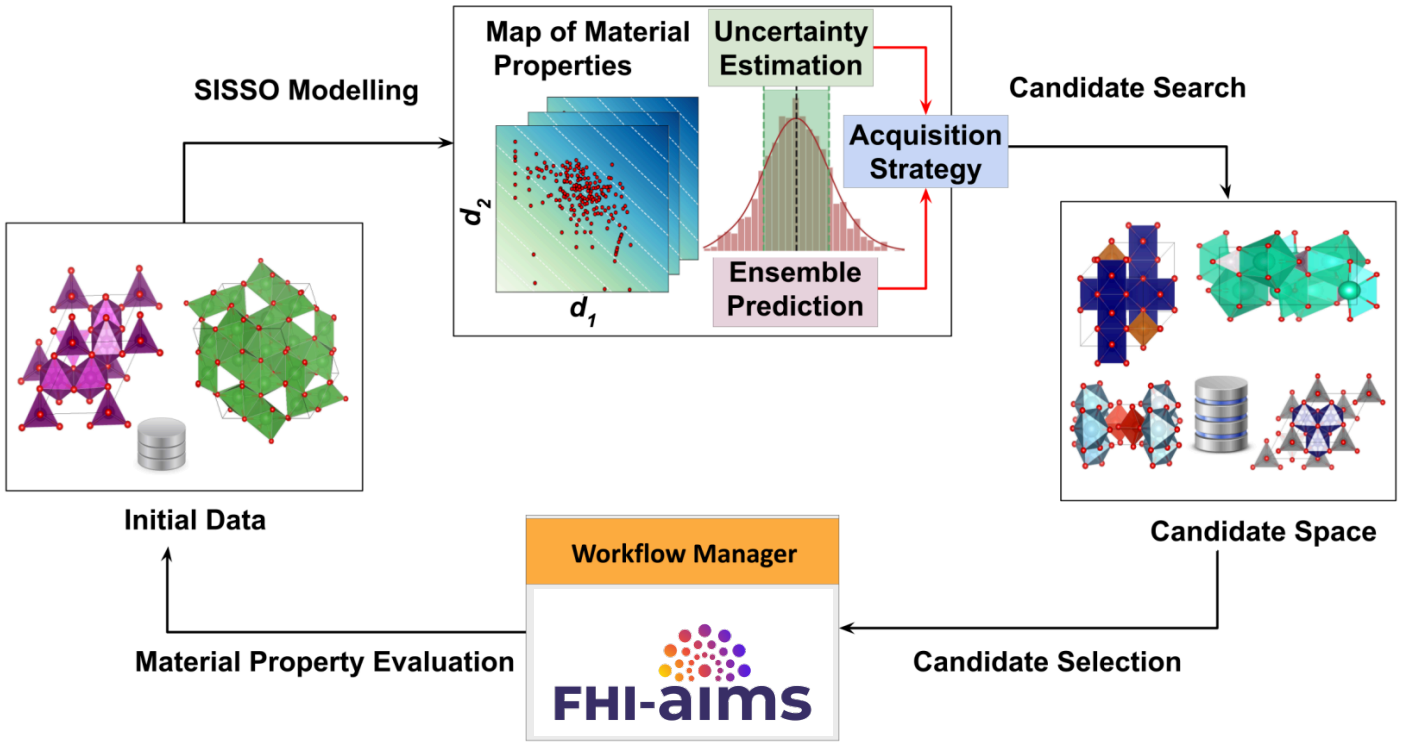
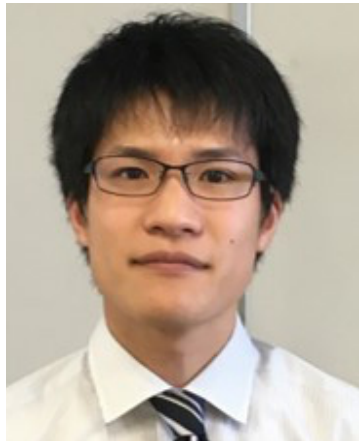
Conclusions

- Consistent Experimental/Theoretical Data + SISSO for Identifying "Materials Genes"
- AI-Guided Workflows Depends on Combination of AI Model and Acquisition Function
- Ensembles of SISSO Models for Quantifying Prediction Uncertainty
- SISSO-Guided Workflows for the Identification of Materials Based on High-Quality Calculations or Experiments



Acknowledgments

Matthias Scheffler



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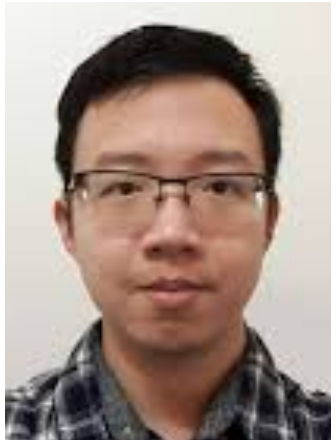

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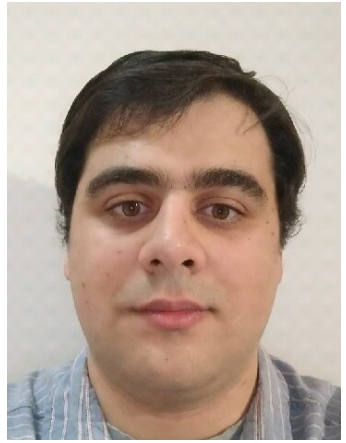

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The NOMAD Laboratory at the Fritz Haber Institute of the Max Planck Society