The High Throughput approach to Computational Materials Design

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Computational materials design

Characterize hypothetical materials using Quantum Mechanics

Existence, Mechanical attributes, Electronic properties, Phase transformations, ...

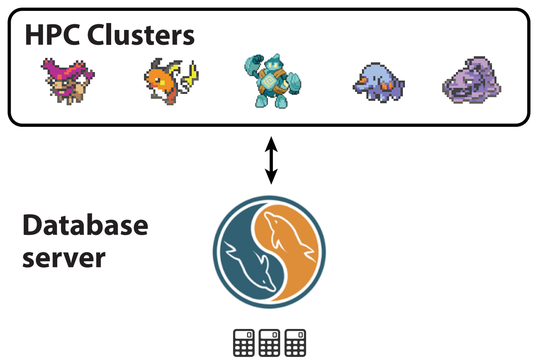
High-throughput screening

Screen a large database of hypothetical materials.

Search for specific targets or discover large-scale trends.

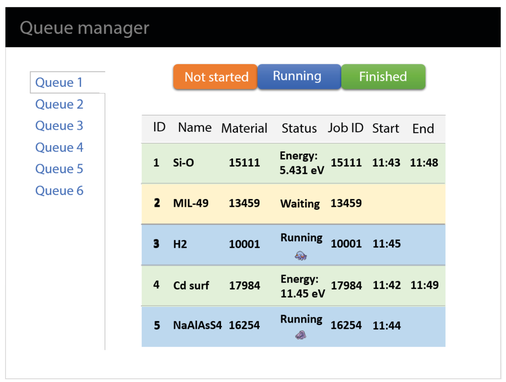
Automating calculations with Queue Manager

External queue with database



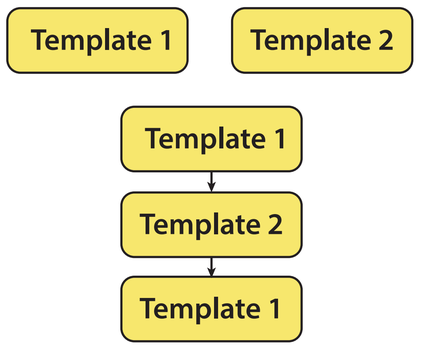
Create, divide and prioritize calculations

Web and app tracking



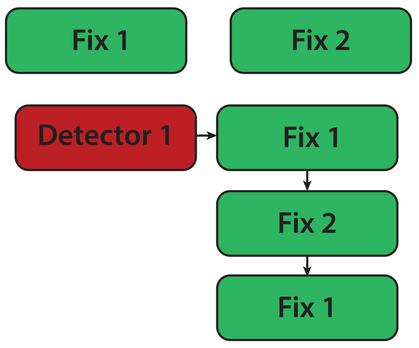
Track calculations on the go

Workflows



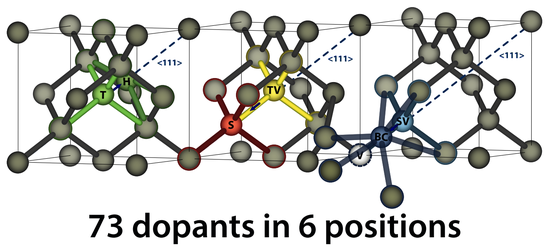
Create calculation sequences based on templates

Error handling



Couple detectors with error workflows

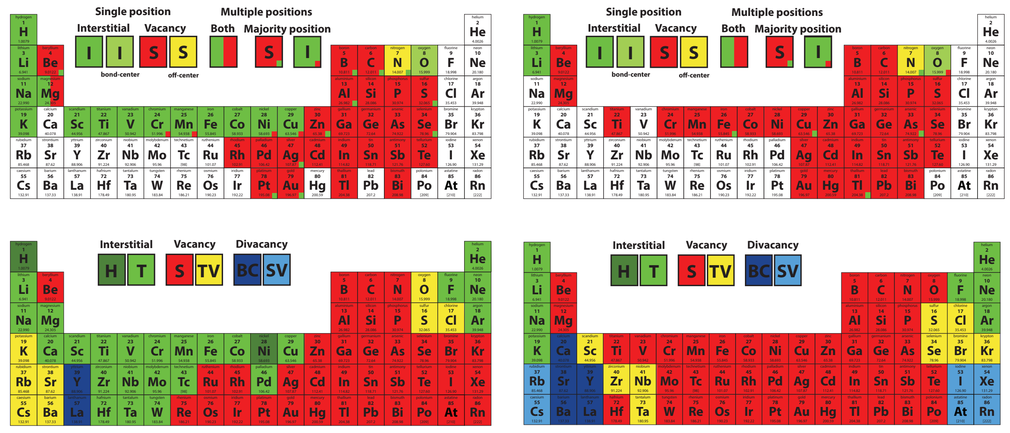
Designing better electronics: Doping Si and Ge



73 dopants in 6 positions for 2 materials

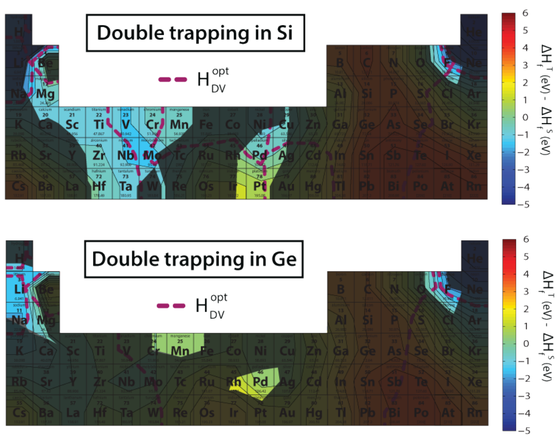
876 materials →~2 calc/workflow (1 nodeday per material)

Positions



Positions are accurately predicted by DFT

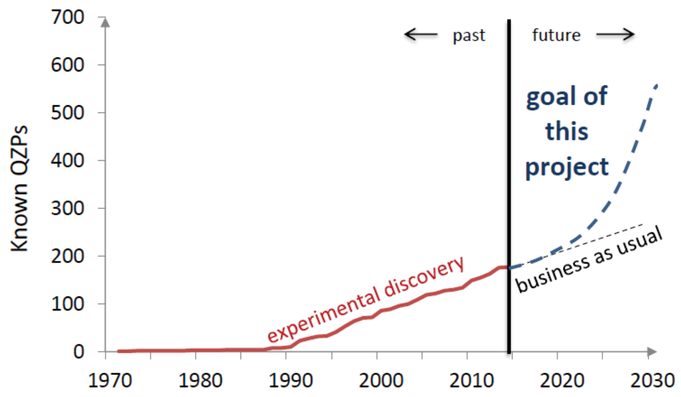
Preventing void formation



Select optimal vacancy traps

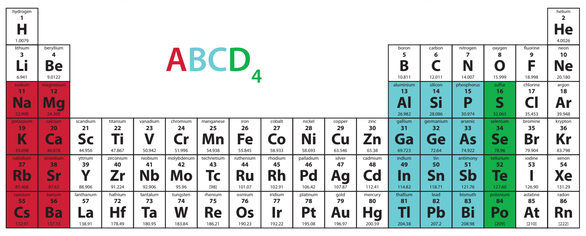
Discovering new quaternary materials: Zintl phases and beyond

Experimental discovery



Less than 10 new materials per year

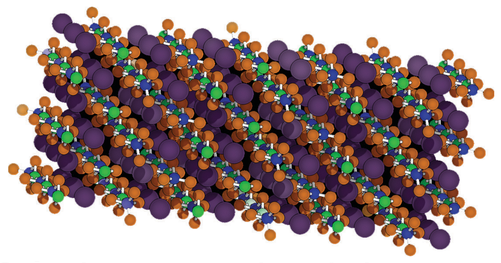
Computational screening set



8 x 12 x 11 x 4 possible materials

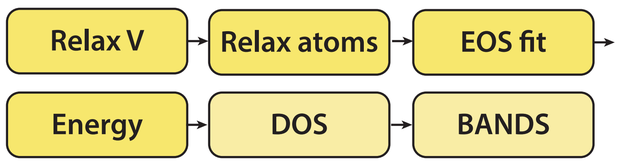
4224 materials ~12 calc/workflow (1 nodeday per material)

Building the crystal



Substitute atoms in existing crystal

Workflow



Stability

Decomposition pathways

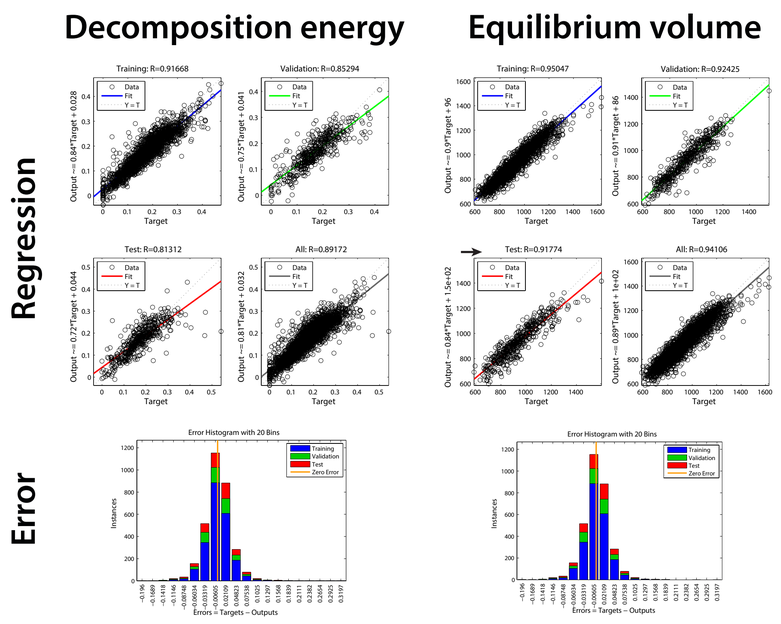
unary: A + B + C+ D
binary: AB + AC+ AD + BC + BD + CD
ternary: ABC + ACD+ ABD + BCD
other quaternary: ABCD

Each combination allows possible energy reduction

114 of 4224 remain stable (6 experimentally known)

Intelligent screening using ANNs

Property prediction based on composition



ANNs learn to convert atomic data to compound properties by learning from an incomplete dataset

ANN → QM priority

Prioritizing best candidates and predicting their output can significantly reduce computational cost

Vlaams Supercomputer Centrum

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