UNIVERSITY OF CAMBRIDGE

OPTiMaDe in Cambridge

Gareth Conduit and Matthew Evans

Materials databases in Cambridge

Cole screening of molecules

Csányi develops atomistic potentials

Pickard for *ab initio* random structure searching

Morris studies energy materials

Conduit deep learning for materials discovery

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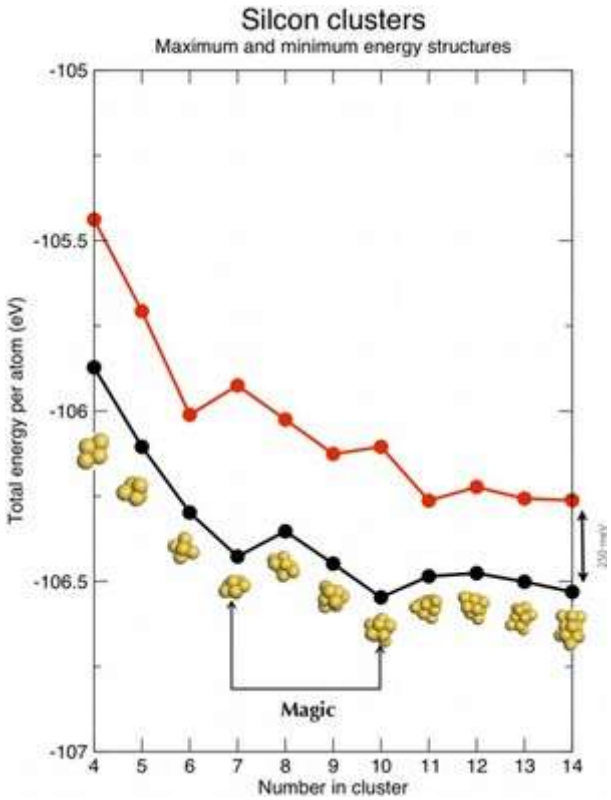
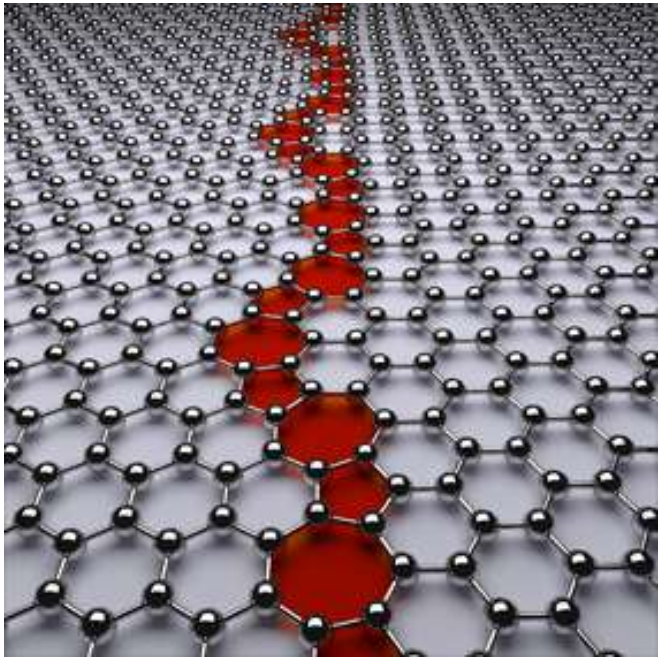
Case study: Pickard group

The next generation database of DFT results for *ab initio* random structure searching will use OPTiMaDe API





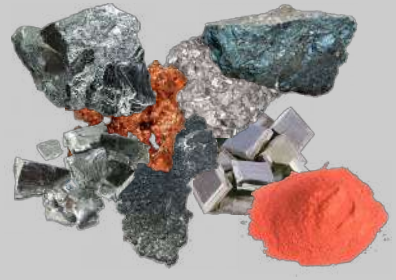
Case study: deep learning in the Conduit group

Deep learning tool to juxtapose experimental data and computer simulations

Use OPTiMaDe API standard for requesting and handling results of computer simulations

Deep learning for materials design

Composition



Properties

Electrical resistance

Stability

Cost

Ab initio

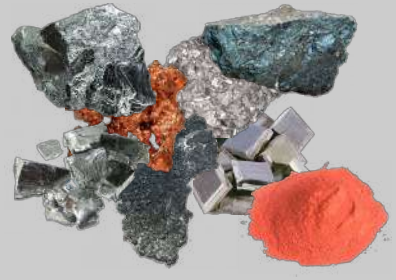
Band structure

Density of states

Phase behavior

Deep learning on fragmented data

Composition



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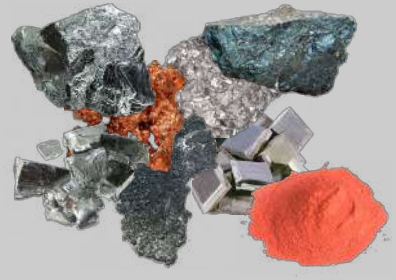

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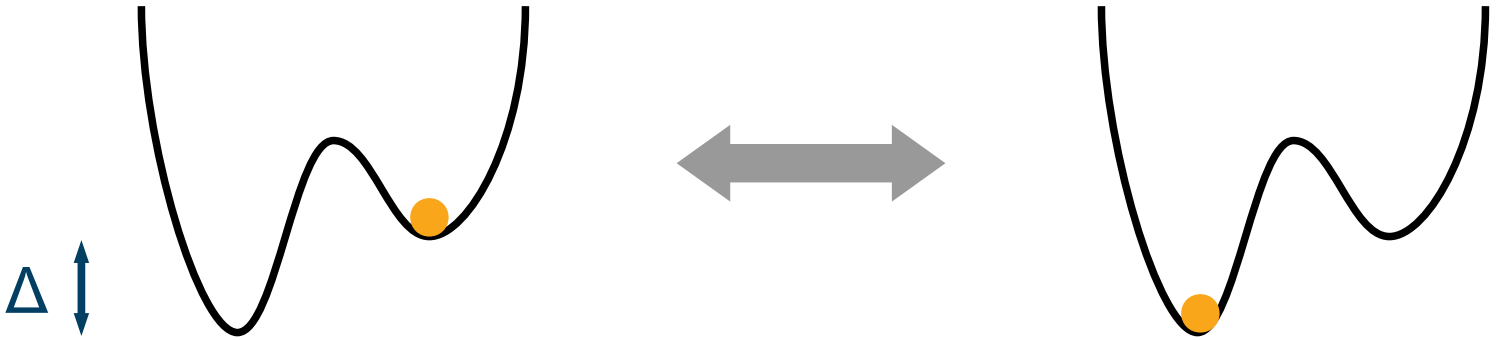
Mechanism and use of OPTiMaDe API

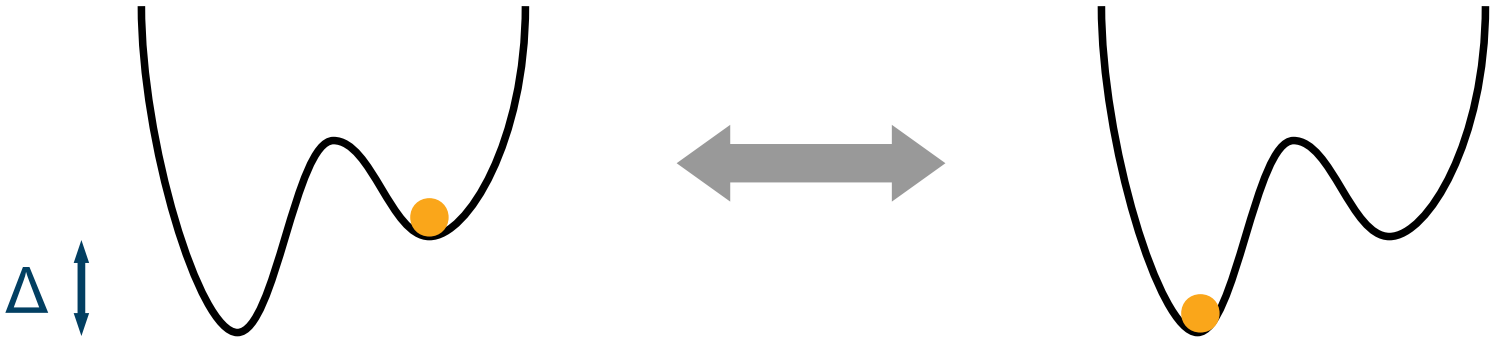
Atom hopping between sites analogous to Kondo effect



$$R \sim \log\left(\Delta^2 + T^2\right)$$

Mechanism and use of OPTiMaDe API

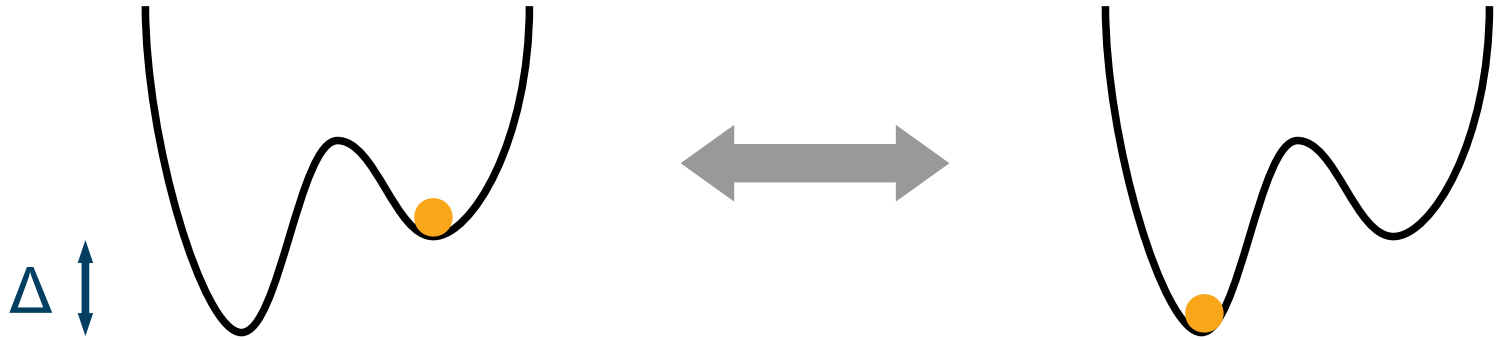
Atom hopping between sites analogous to Kondo effect



$$R \sim \int_{\Delta_{min}}^{\Delta_{max}} \log\left(\Delta^2 + T^2\right) \frac{1}{\Delta} d\Delta \sim \log\left(T\right) \quad \text{for} \quad \Delta_{min} < T < \Delta_{max}$$

Mechanism and use of OPTiMaDe API

Atom hopping between sites analogous to Kondo effect



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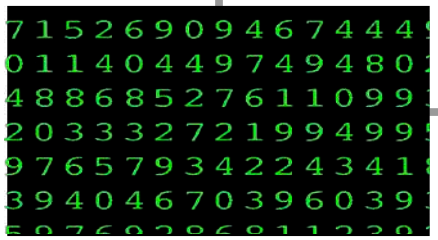
1000 DFT simulations probe the energy landscape and
10000 CALPHAD for phase equilibrium with OPTiMaDe

Merge properties together with deep learning

Flowchart

Request material

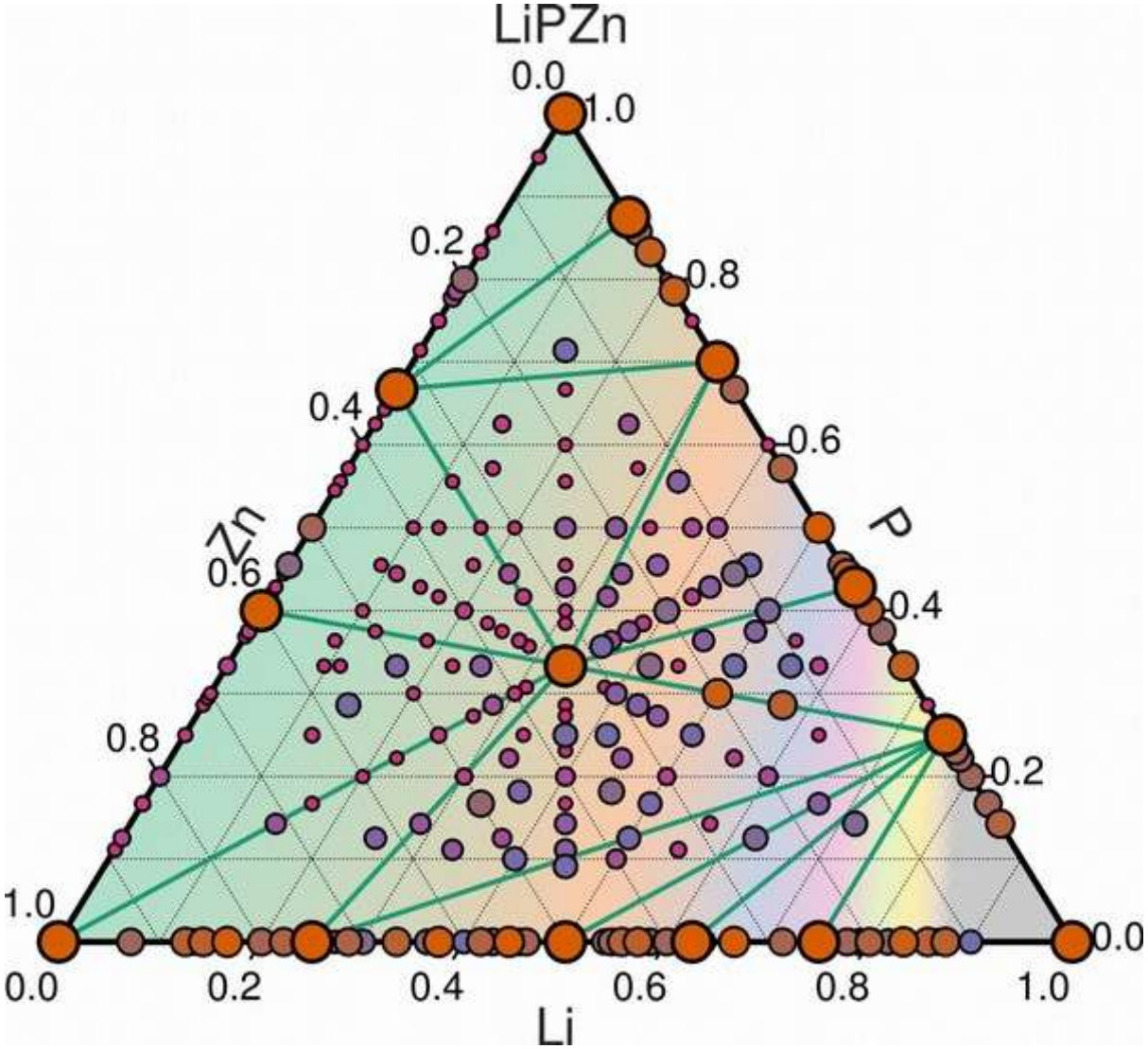


Properties

Example schema


```
{
 "data":
 {
  "description":"phase",
  "properties":{
   "composition":{
    "Au":10.7,
    "Ge":88.1,
    "Ta":1.2,
   },
   "alpha":{
    "Au":7.9,
    "Ge":1.1,
    "Ta":0.7,
   },
   "beta":{
    "Au":2.7,
    "Ge":86.5,
    "Ta":0.2,
   },
   "gamma":{
    "Au":0.1,
    "Ge":0.5,
    "Ta":0.3,
   "solidus":{
    "T":362,
    "units":"C",
   },
  },
 },
}
```

Case study: matador by Matthew Evans in the Morris group



Case study: lubricant design in the Conduit group

Model the viscosity, flash point, pour point, volatility, density, melting point, heat capacity, and boiling point of lubricants

Use deep learning to merge the 1000 experimental data together with 20000 molecular dynamics simulations handled through OPTiMaDe API

Example schema

```
{
 "data":
 {
  "description":"lubricant",
  "nelements":{
   "C":8,
   "H":18,
  },
  "properties":{
   "Tmelt":37.0,
   "Tboil":115.0,
   "C":247.0,
  },
 },
}
```

Requests for OPTiMaDe 1.0

Record the accuracy and uncertainty of data

Provenance tracking to understand relaxation

Incorporate experimental data

Permit material synthesis parameters

Centralized server to query all available sources

Fuzzy searches to reveal all relevant structures

Summary

OPTiMaDe API used in materials design that has led to a novel material for a jet engine blade

Planned inclusion of OPTiMaDe API in matador

API manages DFT and molecular dynamics data for designing new lubricants

OPTiMaDe gaining traction in several groups in Cambridge