UNIVERSITY OF CAMBRIDGE

OPTIMADE Cambridge update

Gareth Conduit

UK Meta Materials Network

UK Meta Materials network has significant support from UK research councils

Interested in developing meta materials database

Planning a workshop in summer 2022 to discuss opportunity

UK META MATERIALS NETWORK

Manuscript on interoperability of materials data for Digital Discovery

Applications of the OPTIMADE API

C.W. Andersen, R. Armiento, G.J. Conduit, M. Evans, Z.-K. Liu, D. Winston

December 2021

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General introduction with a simple example

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Semantic information for expansive/inferred OPTIMADE structures data model (querying non-standardized properties through common semantic definitions) [casper, matthew, rickard]

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[matthew, johan, casper]

1.3 Update on tutorials

[matthew]

2 Databases

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- Remake original table with new rows and update number of results (politically dangerous, but should definitely still be done) [matthew], nice as shows the API is sufficiently stable to allow this

2.2 MPDD

Zi-Kui's database: [Zi-Kui student], run same queries as first paper

2.3 Jarvis

[matthew to approach them]

2.4 2dmatpedia

[gareth to approach them, based in singapore, NUS] +others (check providers dashboard)

2.5 NecrOPTIMADE

[only if exists, Jack Sundberg (related work)] materials resource registry conglomeration [matthew]

3 Future of OPTIMADE

Zi-Kui's use case of MPDD merging of databases [Zi-Kui]
Ontologies for machine learning driven materials design 2021 workshop [gareth, casper, rickard]

4 Application of OPTIMADE to real-life problems

4.1 Machine learning

[gareth and rickard]

4.2 Generative discovery

[someone on the forum?]

4.3 Review of other users

Why are they using it, what do they think, good points and further developments required materials resource registry conglomeration [matthew]
Literature search and review of everyone using OPTIMADE, interface users [casper knows of some] BIG-MAP, the MarketPlace project, DOME 4.0, OntoTrans

4.4 Phase and compound stability

Compare materials stability of combined data (more holistic) versus individual databases (more consistent), will need update to API so can interrogate stability [matthew] - main issue is defining "nonlocal properties" that are computed at some point and will need to updated when new entries are added (e.g. distance to convex hull)

Machine learning case study

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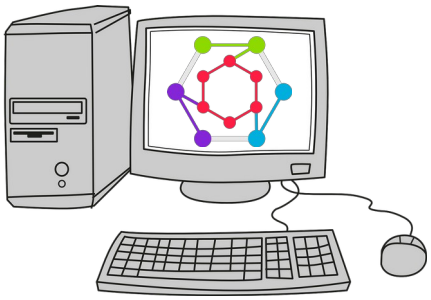
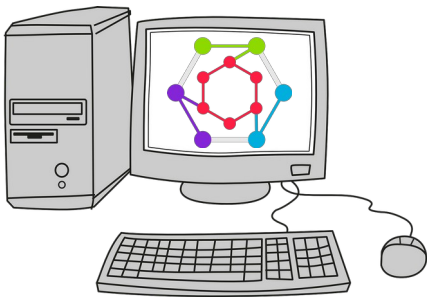
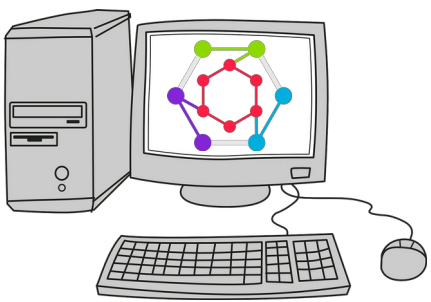
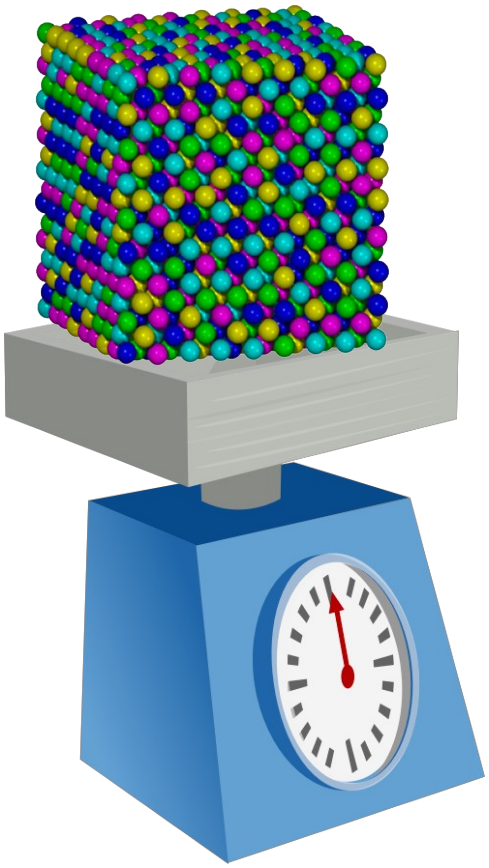
Machine learning merges sparse data









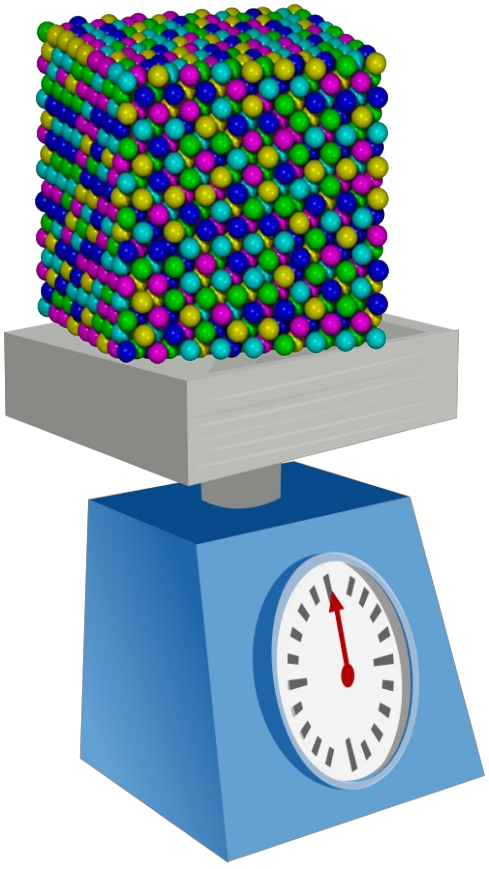
High entropy alloys

Comprise 5 or more elements

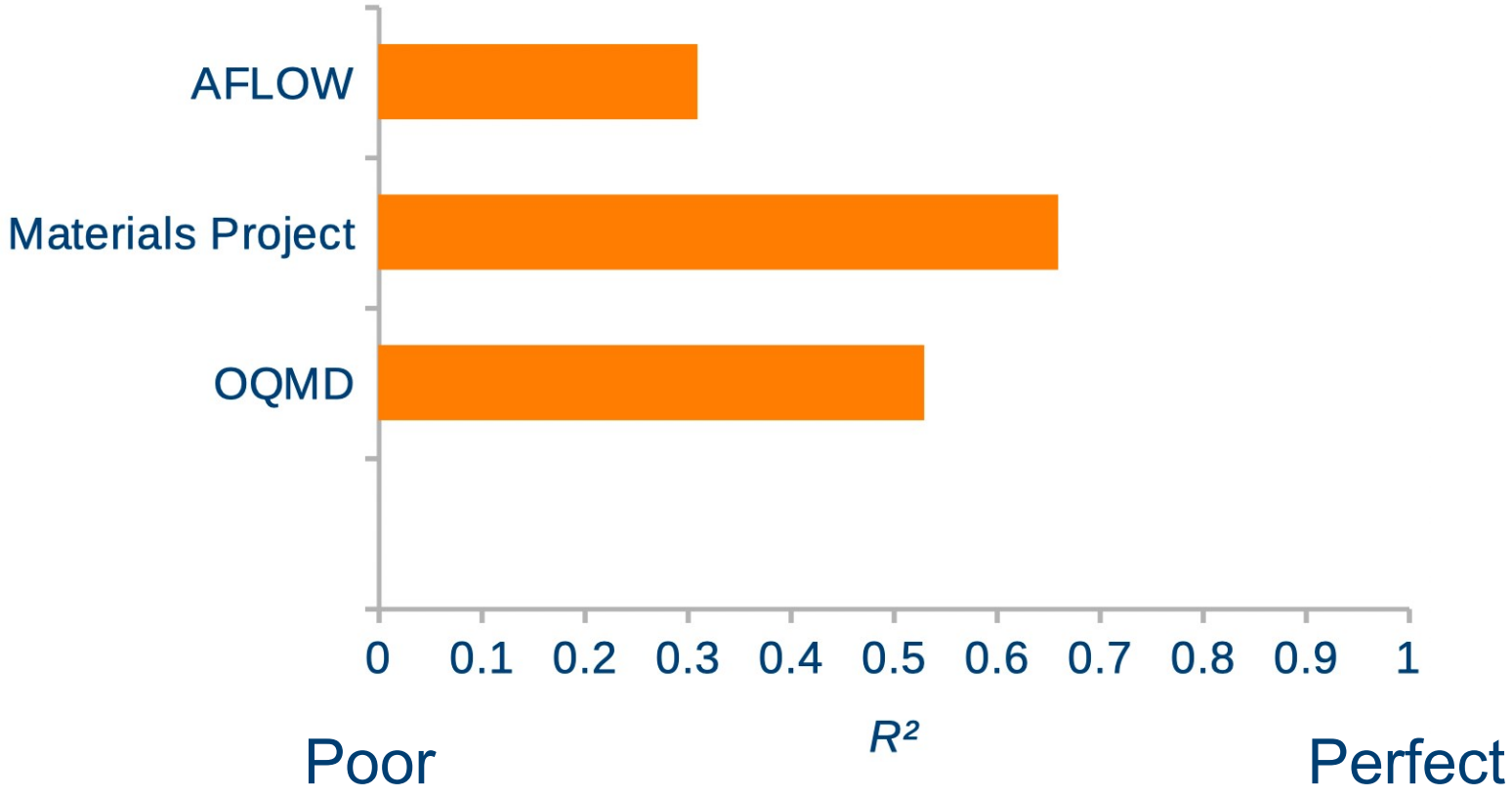
Elements include Mn, Cr, Fe, Co, Ni, Cu, Ag, W, Mo, Nb, Al, Cd, Sn, Pb, Bi, Zn, Ge, Si, Sb, and Mg

Excellent high temperature strength-to-weight ratio

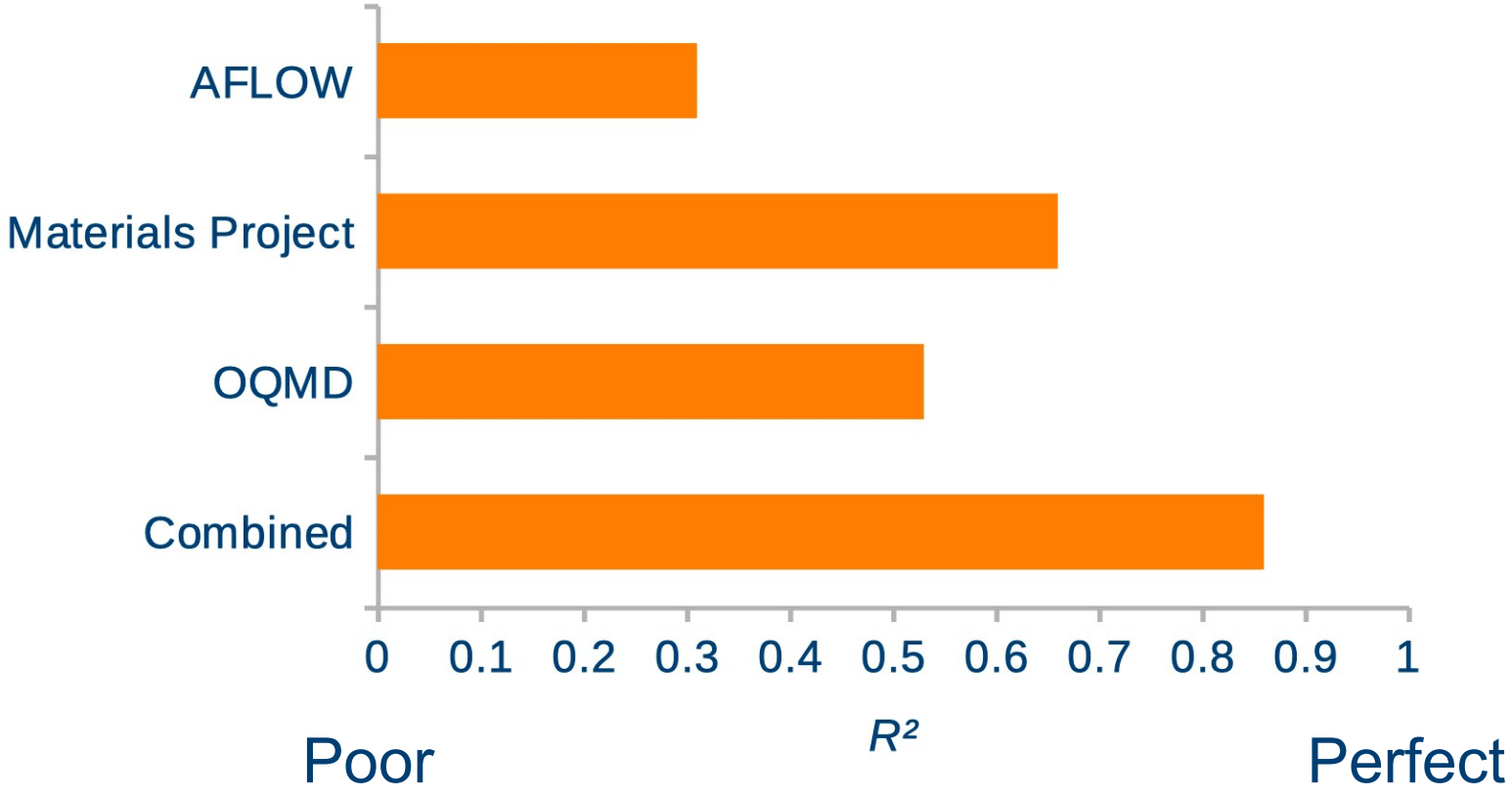
Use OPTIMADE to build a database for machine learning to estimate density



Performance of separate databases



Performance of merged database



Volunteers for other manuscript sections

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