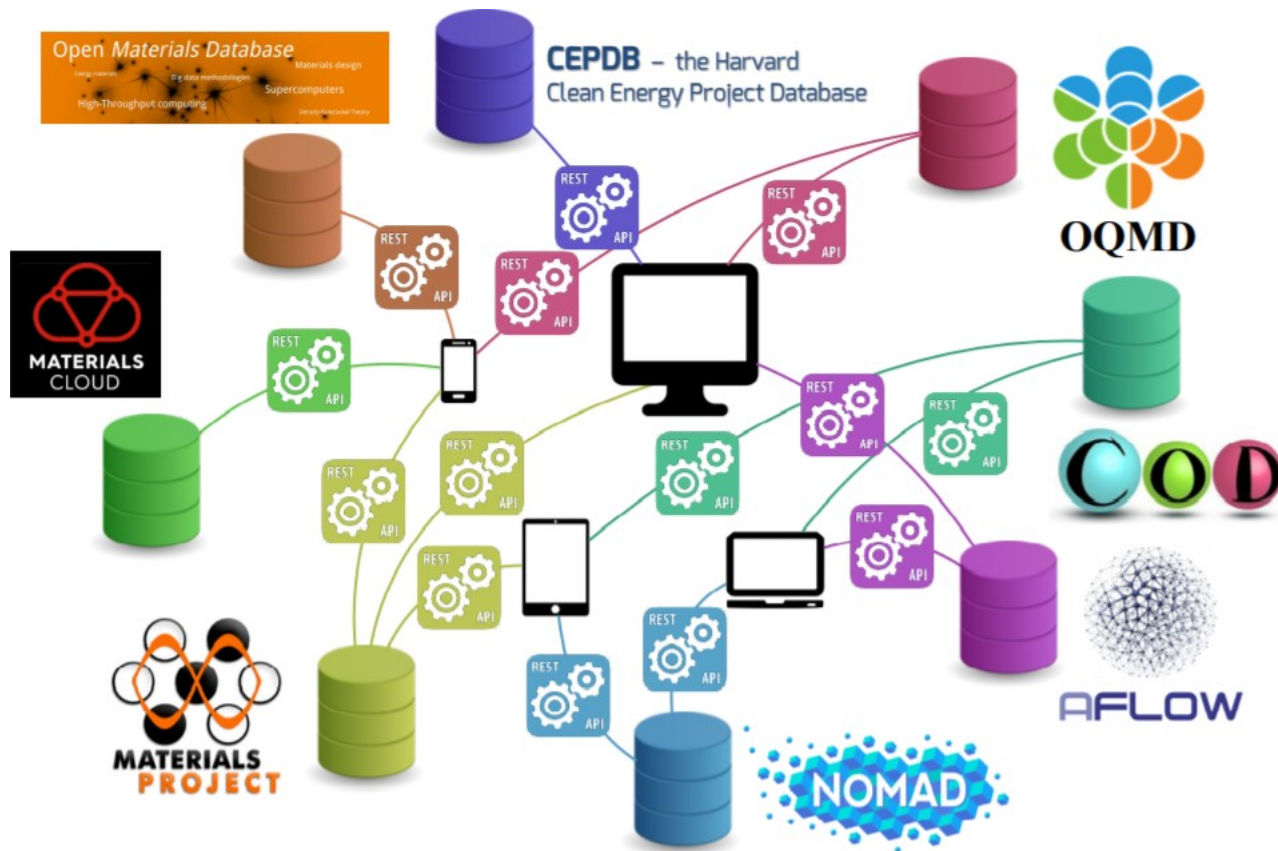


Metamaterials genome: lessons from OPTIMADE

Gareth Conduit

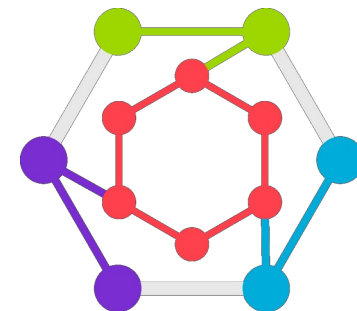
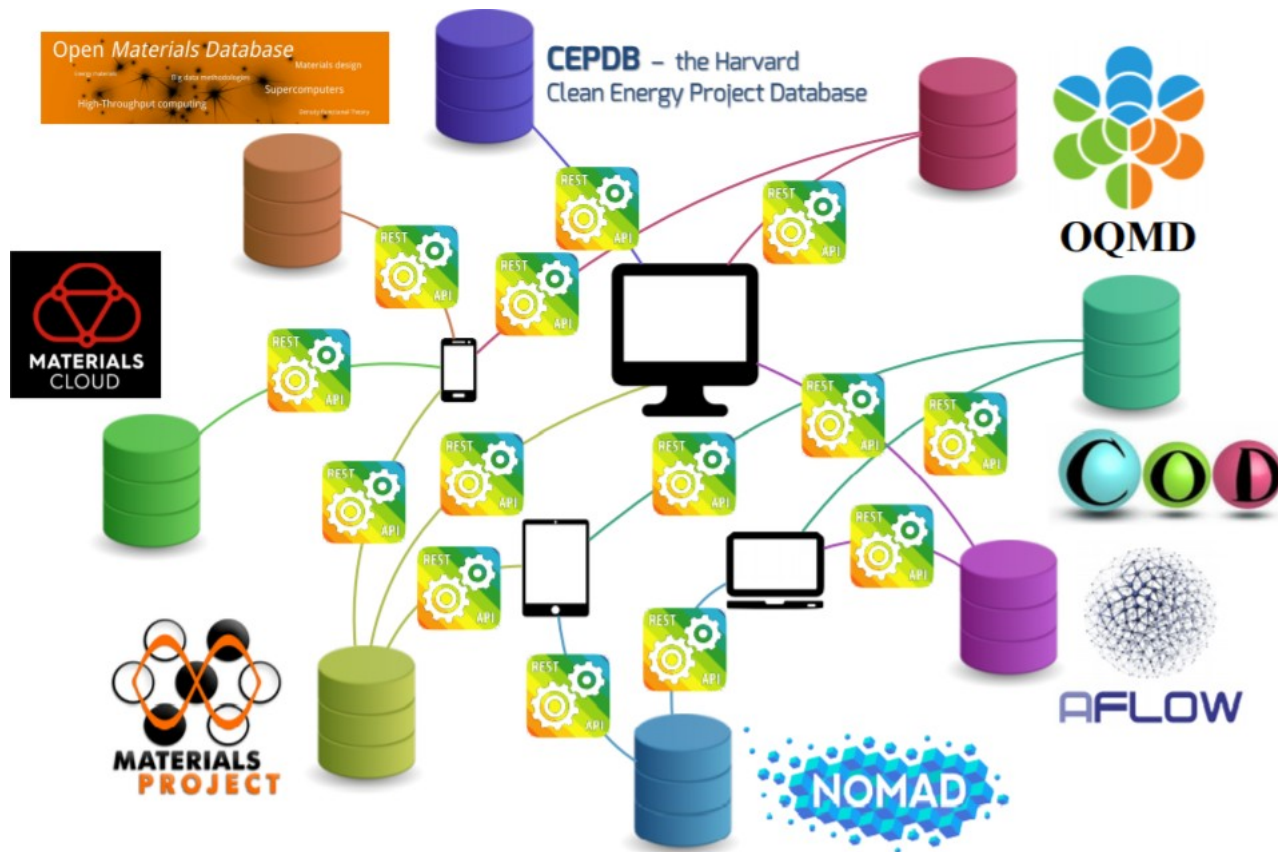
Theory of Condensed Matter group

Data analysis requires extensive access to different databases



Each material database has a bespoke API, an obstacle for machine learning

OPTIMADE defines a common API



*OPTIMADE: an API
for exchanging
materials data*
Nature Scientific
Data **8**, 217 (2021)

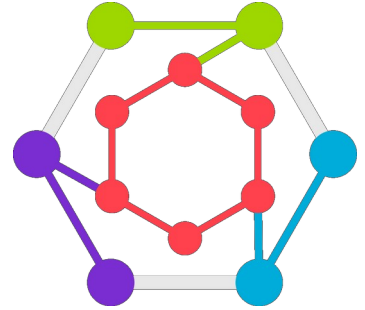
www.optimade.org

2,142,183 structures

python tools provides access to common calls and setup of new client

aflow, ccpnc, cod, jarvis, matcloud, mcloud, mp, mpds, necro, nmd, odbx, omdb, oqmd, tcod, twodmatpedia, aiida, htk, pcod

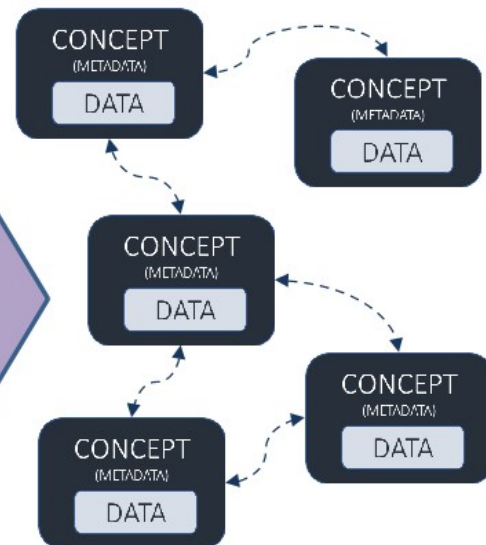
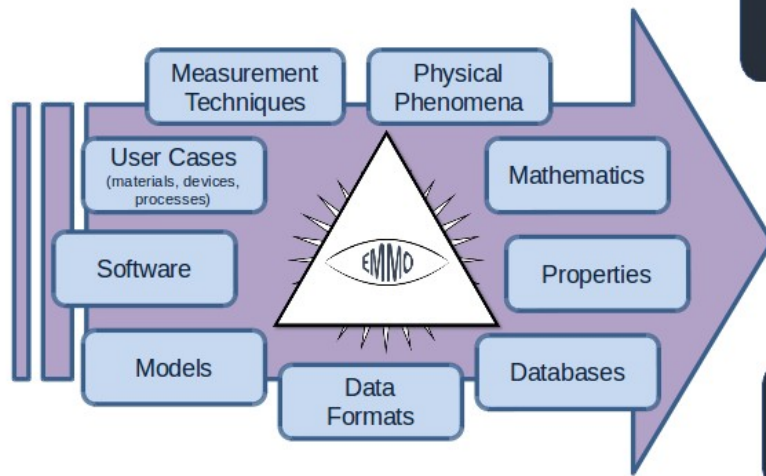
Initially electronic structure, now additional CECAM funding for molecular dynamics





The European Materials Modelling Council

EMMO Objective



USER CASE

From real world entities...

ONTOLOGY

...built on firm physical science, ICT and analytical philosophy foundations

INFORMATION

...to a digital representation.

