

2023-01-26

DPG SKM23 Conference

Hand-written notes wasmer

URLs:

- <https://skm23.dpg-tagungen.de/>
- <https://www.dpg-verhandlungen.de/year/2023/conference/skm/parts?lang=en>
- https://ifffgit.fz-juelich.de/phd-project-wasmer/notes/public/-/blob/main/admin/conference_notes/2023-03-26-conference-skm23/conference-skm23-notes.org

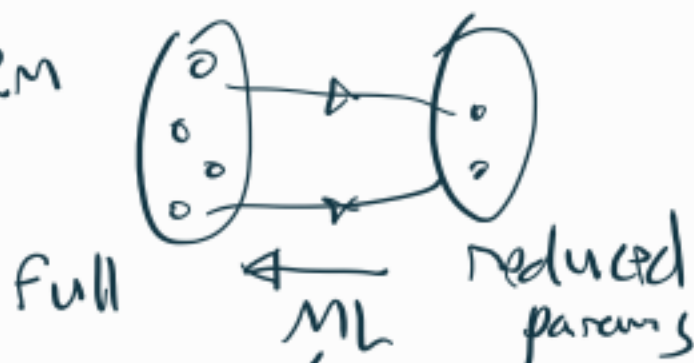
2 Tue 15:15 MA19.2

ML parameter magnetic data single molecule

o) Ligand field parameter fitting ^{susceptibility curves $\chi(T)$} for mole magnets

o) over-parametrization problem

= ill-posed problem



generative model needed



auto encoders
+ "invertible ANs" (2019)

usually only provide one sol, or an average of several. Here, not viable (one-to-many)
2 \rightarrow 27 params

o) Tue 15:00 MA 21.1 |

Abuawwad IAS-1

Materials design topo magnet 2D materials

o) Interesting wrt

QE → JukKR → Spirit

geo/s
optimization

exch
params

mag
GS

used
workflow

o)

3 Wed 12:00 MM29.2 | Lihm

prediction of electron density
& potential with CNNs

init guess

$$\rho_{at} \xrightarrow{V_{Hxc}} V_{at} \xrightarrow{SCF} \rho_{DFT} V_{DFT}$$
$$= V_{ion} + V_{Hxc}[\rho_{at}]$$

ML \downarrow

$$\rho_{DFT} - \rho_{at} / V_{...}$$

$$\rightarrow E_{tot} = \frac{\text{needed add}}{T_{NSCF}} / T_{NSCF} \quad \text{speedup } 2 \sim 5$$

$\rightarrow T_{SCF}$ electron densities

better: $\Delta V_{DFT} = V^A_{DFT} - V^B_{DFT}$

Ronneberger MICCAI2015

U-Net structure, PyTorch

150k params,

516e array, QE

$N=5k$, $N_{tr}=1k$

bFT-at vs mode-at

$V-V_{at}$, $P-P_{at}$

larger error

6 ensth 64 atom

DFT

atomic

ML-J

subst impurity

$$\Delta V = V_{\text{Si 36e}} - V_{\text{Si 64}}$$

Si 64

$$\Delta V_{\text{ML-V}} - \Delta V_{\text{DFT}}$$

$$\Delta V_{\text{at}} - \Delta V_{\text{DFT}}$$

WF basis

check for artifacts due to up sampling
from con

Problem no LR effects = screening + electrostatics
due to small unit cell

AC:

validate
with

b) $E_{\text{pot}} \in H$? that is real validation

c) My Q: SdNet upsampling
→ Continuous convolutions

d)

o) 3 Wed 12:15 MM29.3]

Chem ordering & magnetism CrCoNi alloy

Ghosh et al. PR Mat 6, 113804
(LRPs) + MC 2022

"magnetiz" MLIAP (Shapeev)
(really, brute-force statistical
approach. But how in comp spin?)

Du et al Acta Mater 2022 MC/MD/NNP

KKR-CPA/MC

Woodgate PRB 2022

Cr/Co
alloy

(collinear only)

o) 3 Wed 12:30 MM29.4

Rinaldi

charge-dependent ACE

Lit to include electrostatic interaction

Q_{eq} P_{model} 1991 Rappe

1 Ghaseini 2015 B92

2 Ko et al Nat Comm 2012

3 Grigati 204705 2019 | SOAP, LOVE

4 Gao Comm B 1572 2022 | Wannier centers

5 Zhang Phys 156 124-107

Here: Q_{eq} into ACE

$$E_i^{ACE} + E_i^{QPA} + E_i^{elec} = E_i(r)$$

Implm in pacemaker

$$\text{loss } L = \sum_n \sum_i (q_{in}^{ACE} - q_{in}^{bFTZ})$$

↳ charge equilibration
for case when charge not exply
fittable.

3 Wed 12:45 MM 29.5

MLIP silica nonlinear ACE

Erhard NPJ M890 22

2022 used GAP
now exist "much faster" pots

Now active learning for MTP,

VASP + SCAN

→ nonlin ACE

faster convergence
using different embedding theorems

Active Learning:

compression, anomaly, querying

small scale plus large scale, refit

→ 11K structures 1 mio atoms

split 0.05

d) CALPHY comparison

6) 3Wed 17:15 MM31.6]

Active learning accel HTC mat search

Pwcell - Active Learning
SISO++ implmtn OS software f(2022)

tinyurl.com/sissopp

3 Wed 17:30 MM31.71 Botti

ML Discovery New Materials

a) Perovskite ABC_3 stability # ternaries
SO cwrdat.ehu.es # quaternaries

& Schmidt 2017 500k compo
quaternary ABC_2D already 13 Bio.
mio 5 mio s.
reals

a) Schmidt 2021, 2023 large ~~GAT~~ IN
CGATs
[tddft.org/bmg/...](http://tddft.org/bmg/)
↳ gallery
1 large model
62 M params
4 mio = N

Q&A J. Margraf

o) 3 Wed 17:45 MM31.8 | Lokamani

MLAP magneto-elastic TM alloys novel phases

o) USPEX Fe₄Ni datgen

$\Sigma 9 \dots 100 \text{ GPa}$

o) SNAP Descriptor FESNAP/DAKOTA

o) Lspin-aware MLAPs \rightarrow (Heisenberg Halm)

Via LAMMPS simulation

(Heisenb Ham subtracted, simulated with pot
(that way becomes spin-aware, or sth))

o) 3 Wed 18:00 MM31.9}

Sellschapp FAIR HTC screening
"Knd:4Mat > AiiDA"

6) 3 Wd 18:15 MM3A.10

D-ML C₅₀H₁₀₀ molecular
crystals

4 Thu 10:30 MM 36.2

ACE with domain knowledge

1) parse, describe, BOP Fox ^{CN polyhedra}
Hammer Schmitt

Fe-Mo binary system

↳ enumeration of all phases
(there are a lot)

Magnetic & norm

use RFS recursive feature selection

several regressors → weighting regressor
(average)

seq. FS

CNAV = averages of CN polyhedra
improves SOAP, ACE, ...

+ KRR / RF / MLP / ...

o) 2 "convex hull" & DFT "what is this about?"



It's just E_{form}
vs alloy concentration)

4 Thu 10:45 MM3 6.3

ML framework for equivalent atoms at surfaces

edges, corners, kink, adatoms, vacancies, ...

↳ put into "equivalence groups"
multi-species

SOAP_{cut} $\approx \sim 2NN$ species χ_i

dim red MDS $\|\chi_i - \chi_j\|_2$ $\begin{matrix} \text{dim} \\ S' \leq S \\ \text{now a} \\ \text{hyper} \end{matrix}$

mean shift clustering used
 $S' \leq 2$ Emb dim

check: $\chi_{im} = CN$ number ✓

self-adjusting hyperparams in ML cycle

gitlab.mpcdf.mpg.de/Klari/decaf

6) 4th 11:00 MM 36.4 Saxena

Use Autoencoder to visualize SOAP space
for informed hyperopt

going back to encoder space invertible

o) 4 Thu 11:15 MM 36.5] Ibrahim

ACE MLIAP transferable water/ice

4Thy 12:00 MM 36.7] Larger
Graph ML Potentials in JAX

github.com/sirmarcel/glp (TBA)

d) 20~~22~~²³ arXiv Rupp
Green Kudo AD

e) 503 Kates MLJAR
= stretched down version of NequIP
~ 10% of params → faster