

A1.01 Strictly constrained neural network exchange correlation functionals (Ryosuke Akashi)

A1.01 Nagai 2018, 2020 ML-DFA
2022 V_{xc}
repr

Idea $V \rightarrow V$ mapping

$$n(\zeta_i), i \in N_c \rightarrow E / V_{xc}(\zeta_i)$$

But that leaves out all
 $\zeta_j \notin \zeta_i$?

Incorporating exact constraint to
satisfy ^(exact asymptotes) analytical solutions like HEG.

→ Stable convergence ("physically constr. NN")

"Applicable / extendable to any kind of constraint(s)."
/sets

New developments in quantum Monte Carlo simulations A8

Gaussian Product States: Datadriven wave functions for correlated electronic structure George Boo

Bridging Bayesian ML & QMCP
(sim. Foulkes, real space approach)
= Kernel ML

Application to frustrated spin systems
then fermionic systems

Analogy: config space \leftrightarrow 2D Image Recognition
 $\left(\begin{array}{l} \text{pixel} = \\ \text{el. in \ß} \\ \text{state or not} \end{array} \right) \quad \left(\begin{array}{l} \text{pixel black} \\ \text{or white} \end{array} \right)$
 \rightarrow sample large phase space

Materials discovery by high-throughput screening and artificial intelligence B8a

What can we learn from machinelearned physical relationships?

Luca Ghiringhelli

1) Reg Learning \leftarrow ^{DL} "symbolic inference"
just refashioned SISSO?
(but also see symbolic ^{DFA} ML)

2) SISSO Recap, Multi-SISSO

Informtheo feat Seltn

3) BRegler Scheffler 2022 TCMJ

Mutual Information; fspace size not limited.

4) Symbolic regression interpretation

B8.07 Exploring structure-property maps with kernel principal covariates regression and chemiscope (Guillaume Fraux, B.A. Helfrecht, R.K. Cersonsky, M. Ceriotti)

PCoVR : allows mixing ^{props info} ^{w.} ^{structural info} ^(wrt) ^{struct-prop map}
 tunable via $\alpha \in [0,1]$




latent space

KPCoVR

B8.11 McLoughlin

- ~~27~~ Tins
- i) topo DB : "Materials" and "T.M."

Nature ~~26~~ 566, 435 2019
Non-magnetic

- ii) Benchmark classification 
- RF, AutoMatminer, MobNet, MEGNet

Tuesday

Diagrammatic many-body theory A2a

A2.15 Machine learning density functionals from the randomphase approximation (Stefan Riemelmoser, Carla Verdi, Merzuk Kaltak, Georg Kresse)

ML-DFA from RPA

• RPA-OEP ^{= "true" local xc fctal} optimized eff pot
↳ costly \rightarrow ML

• \rightarrow "ML-RPA"

using 2-, 3-body descr from

MLPs for expansion of $n(r)$

use coeffs as descriptors, make
rotinvar. ML: KRR.

• "we have all the pot data in realspa
making us more data-eff"

-) systems: VASP DFA implem
 $O(N \log N)$ scaling
 diamond, surface states
 graphite, vdW interactions
 H_2O MD

Q&A

-) have two stay w. same pseudopot
 once chosen for training
-) rotinvar: $m(\mathbf{r})$ should stay
 the same when you rotate your
 coord sys but a vector should
 be
-) Incomplete descriptors: (2,3 body, finite cutoff)
 tried 4-body,
 no imprvmt
-) not expensive? no since FFTs compute
 at every point

LINK: SALIED

-) R_0 : reduce $O(N^4)$ of $(ij|kl)$
4-body el rep integrals by

repl. $\psi_i \psi_j$ products w. auxill basis fcts $\rightarrow O(N^3)$.

Applications in QCh, GW.

-) c0hl: can express polarizability in GF $O(N^3)$
-) Impl in FHIkins, NAOs atom-ce orbs
separable R_0
- *) Error < 1 meV or better cmp to GW

C5.03 Nonunique fraction of Fock exchange for defects in
twodimensional materials (Wei Chen, Sinéad M. Griffin, Gian-
Marco Rignanese, Geoffroy Hautier)

TMDs

-) hybrid Funtals \rightarrow GKC Koopman
for accurate defect levels in 2D mats
-) WSe_2 calc: $G_0W_0 \xrightarrow{+@PBE} \sim 2.8 \text{ eV}$
 $+SOC$ band gap
-) Fock exchange α_K as SAT checker for
GKC
-) checked for different defects:
 \nrightarrow ^{GKC} always violated
-) std hybridals fail for these systems
due to reduced screening defect host band
edges

- o) Kagome lattice systems
- o) AV_3Sb_5 ^{monolayer} \rightarrow s-wave supercond
symmetry breaking effects
- o) VHS van Hove singu
- o) TRSB CDW \rightarrow AHE supercond
Time reversal sym break

C5.29 HTC stacking of 2D vdW materials

· vdW heterostructs, twistronics, slidetronics

o) Database: C2DB ~~4K~~ 4K monolayers

· sophisticated stability analysis, workflows, exploring stability landscape (saddle pts, min, max)

o) ^{other} DBs, "natural stacking" = bulk: ccd/icSD, Bilayer DB.

DFTB parameters for the periodic
table, part I

Chiara P. ₁ $\{\epsilon\}$, ₂ $\{U\}$, ₃ $\{\epsilon_{\text{conf}}\}$,

₄ $\{\epsilon_{\text{rep}}\}$ & black magic
TODO: contact

Johannes Margraf

→ parameters for the PTE

(Chiara: only for 1-3,
for 4 "will never work")

(1-4, 4: $\hat{=} v_{\text{xc}}$ in DFT)
DFTB

1) Finding powerful variational
reps



2) Neural QStates Carlo Trojer 2017

3) Today: Fermions (past: spins, bosons)

→ 2nd Q
JW mapping → map onto spins
BK mapping

4) Correl ^{mb} groups same as FermiNet (MFOULKS)
for exact sampling
5) recent pub: veerapaneni 2022 arXiv

6) Other Approach: 1st Q "Hidderfermbs"
consistently via augmented
2) Better than backflow rep Hspn
(Hubbard model, tested on)

3) Application to nuclei

4) Net Ket

- AB_2X_4
- Props =
- 1) Bandgap & mixing energies via cluster expansion of the bandgap
 - 2) Descriptors: Cluster Correlation Function (CF)
CM, MBTR
 - Models: LR, ML Perc, GBRF
 - 3) SHAPley value analysis:
 - 4) Twitter @pablos-pv
 - 5) Q&A

(BIG-MAP) (Δ -ML)

-) **TODO: finally understand Δ -ML**
"FJK/HF/STO-36 for Δ -ML"
-) "FJK rep" of Slater from HF + KRR with kernel K_{Slater}
$$K_{\text{Slater}} = \sum_i \sum_j K_{\text{orb}}(\phi_i^A, \phi_j^B)$$

for extensive props ($\frac{\text{tot}}{\text{ref}}$)
-) For intensive props (HOMO)
-) Tests on QMG cmp with CM, ...
Qint-T — here "heavy atoms"
LIBE = Li cations
-) target el. energies
-) costly

Strong spin-orbit and magnetic systems C9

Hidden order and magnetic
excitations in spin-orbit double perovskites

Leonid V. Pourovskii



- 1) correlated insulators \rightarrow degen d/f-els \rightarrow multiple moments
- 2) DFT + Hubbard $-I$

Missing: superexchange, RKKY

\rightarrow post proc: LinResp

\rightarrow yields full set of intersite exch interactions,
($|E|$) (J_{xx}, J_{yy}, \dots)

\rightarrow hidden order = ferro-quadrupolar xyz phase
gen. by superexchange

\rightarrow from $H_{\text{eff}} \xrightarrow{\text{use}} \text{GS } 1\text{-el densmat}$
as starting guess for DFT+U.

A5.15 Benchmark of density functional theory for superconductors (Mitsuaki Kawamura, Taisuke Ozaki)

6) Framework SC-DFT

~~LDA~~ \rightarrow KS-PT (eg OEP) \rightarrow VASP, pseudopotals

$\Omega[\rho, \chi]$ order param includes
SOC, phonon interact, BS, ...

*) order param $\chi(\underline{r}, \underline{r}') \equiv \langle \psi_{\uparrow}(\underline{r}) \psi_{\downarrow}(\underline{r}') \rangle$
 \rightarrow Eliashberg-combined f.tal 2020

*) screened exchange, spin fluctuation
 \rightarrow need augmented charge
 \rightarrow Vanderbilt ultrasoft potentials

a) Benchmark for elmt crystals
"Superconducting Tool Kit"
SCTK

daydobr2020

Eliashberg-combird Summer 2020

b) Summary

SOC plus SF (fluctuation)

SF essential for transition metals

SOC is small for elmtl systems

A5.22 2D superconductivity driven by electron-phonon coupling at the interface with the charge-ordered semiconductor BaBiO₃ (S.Di Napoli, ..., Verónica Vildosola)

- BaBiO₃ perovskite with BaPbO₃ layer on top
BBO BPO
-) El-Ph coupling causes high T_c
 -) semi-local DFAs, cheaper, since dense k -mesh needed
 -) 2D SC observed exp 2017 Augsburg
Goal here to explain it.
 -) charge transfer from Bi₃₊
 -) Calcs: VASP of course, HSE, GGA.
 -) DOS tuning: thicker BBO, larger T_c

A4.07 Charge transfer through defect states in TMDC-graphene heterostructures (Daniel Hernangómez-Pérez, Andrea Donarini, Sivan Refaely-Abramson)

•) vdW heterostructures

emergent behavior from stacking of different 2D layers

→ sequential el transfer, light harvest & emitter, ultrafast charge transfer

•) Strong confinement

•) System: WS_2 - Graphene

∃ an electron in the vacuum why?

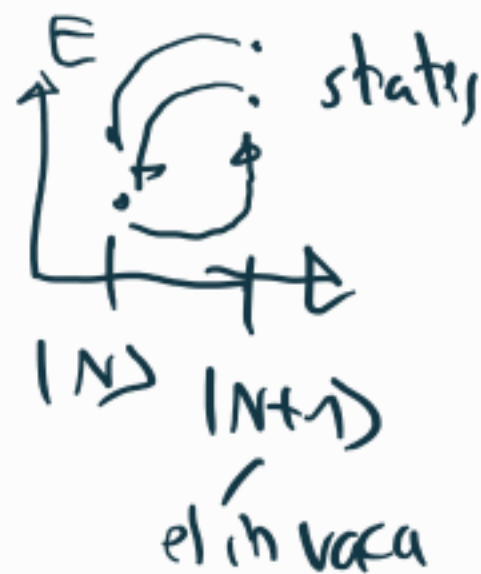
Flat defect bands by bridge w graph layer
"Typical"

•) Transport Model: $\hat{H} = \hat{H}_{sys} + \hat{H}_{lead} + \hat{H}_t$

incl SOC (\equiv SOJ)

Master Eqn for transition rates

b) SOC & magnetization
shows BS. At $\bar{K} \rightarrow$



c) Summary

VACANCIES in X_2 -graph

source of non-trivial dynamics

d) DFT, \hat{H} , ME formalism \rightarrow transition rates

Wednesday

Topological properties... C8a

Topology: a New Periodic Table of Materials, Classification and Interacting Flat Bands

Bogdan A. Bernevig

1) Overview: ↗

2) New stuff: Flat bands, ...

3) (new terms: gapless hinge states, ...)

4) Classification of non-topo insulators: atomic & obstructed atomic insulators (OAI)

in terms of bands, topo effect is in terms of symmetry of BS eigenvalues

5) Search for supercond in flat bands

6) Flat bands & Twisted [bilayer] mats

7) Interacting Model, now with heavy

Fermions / Anderson model

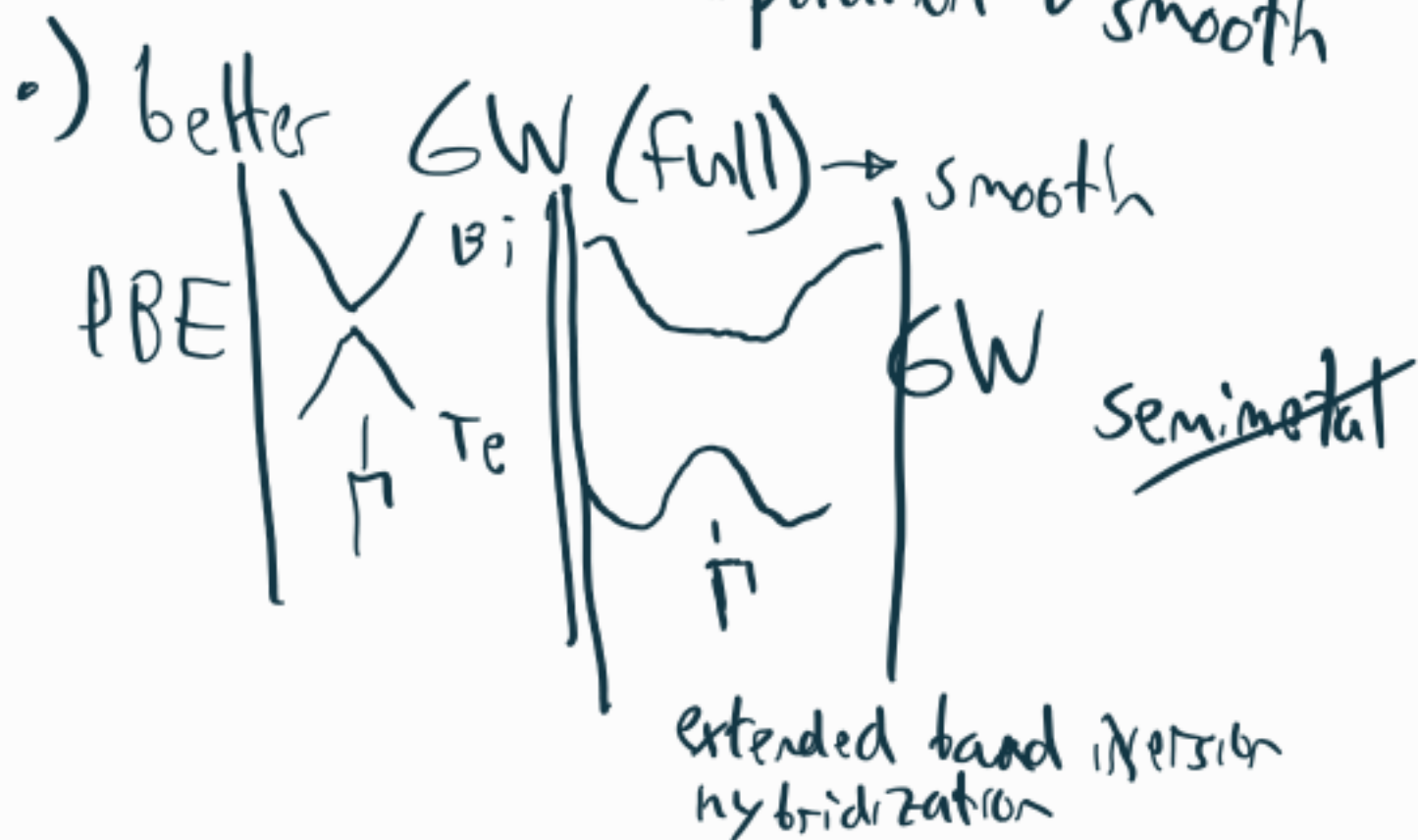
•) from start: bilbao crystal server for
Magnetic materials.

•) "fragile topology"

•) traditional classification: Zak 2001

C8.01 Bulk and surface electronic structure of Bi_4Te_3 from GW calculations and photoemission experiments (Dmitrii Nabok, ... Irene Aguilera)

- 1) DFT not enough, need GW (semimetal)
- 2) GW has problems (unphysical spikes in BS from off-diagonal Σ^{SE} terms)
need Wannier interpolation \rightarrow smooth



o) GW (full) \rightarrow Wa Int \rightarrow Calc Topo Indirect
 $\frac{\gamma}{2} = (1; 111)$
 $\sum_n = 1$
 \rightarrow Nakai 2022
So, a SG + TCJ

o) Semi-infinite film calc GW (full)
with QL, BL (quintuple, bilayer)
w. Wannier Tools

o) Comparison with ARPES photoem exp. ts

o) Summary

o) Bi₄Te₃ indirect band gap semimetal

o) dual ^{is a} topo mat

o) Need GW (full) effects \rightarrow band gap opening

Machine-learned surrogate models: the quest for ab initio accuracy at a fraction of the cost B5a

Blurring the lines between electronic structure and machine learning

Michele Ceriotti

•) Unified AML Theory

→ Poster, B5.39, B5.25

•) Munsil 2021 Recap

esp completeness = injective cf. ↑ poster,
plenary talk (Sanyi)

•) Feature Constr

- fully equiv: NICE

- long range: LOPE

- MPN, N-cent: MP-ACDC

// nice viz of general baseless
neighbor-density correl fun
"decorate" with sth

eg SH to describe
props that transform
like SH.

•) Applications: ¹⁸ shiftml.org
 ¹⁹ alphaml.org
 :

-) Combining structural & functional props
→ bigli, Veit et al.

eg predict phase diag & prod sth simultaneously
eg other examples 2019-2021 well-known

-) ^{Moving} From data- to physics-driven

eg Mahmoud, MC, arXiv ... 91

•) What next?

•) Software stack for ML

•) Hands-on session MARVEL booth
Thu 15-16 pm

•) Experimental data

Slides: ~~tigut~~ Cerrothi - prisk22

B5.53 Bypassing the cost/complexity tradeoff in atom-density potentials (Claudio Zeni, Kevin Rossi, Andrea Anelli, Aldo Glielmo, Stefano De Gironcoli)

-) BPNN, GAP, MFF/FLARE, ...
nonlin Fixed rep
-) lin fixed reps: ACE, SNAP, MTP,
-) nonlin ReLearn: NequIP, GemNet
Graphormer, PaiNN, ...

(of lin pots)
•) Problem: Incr speed w/o. sacrifg acc
Soln: "Div & Cong Potentials"

Take many models \rightarrow weighted sum
Smooth interpol, model weights
eg soft max (also said
centroid, cluster)

b) Results

- ✓ consistent improve acc to add cost
- active learning
- ✓ use model weights to tune a baseline pot

aka.ms/A14Science
"Jobs"

B5.01 ML approach for longitudinal spin fluctuation effects in bcc Fe at TC and under Earth-core cond. (Marian Arale Brännvall, D. Gambino, R. Armiento, B. Alling)

In bcc Fe at T_c

SPF



LSF term
for $T > 0$

c) ~~was~~ $H = - \sum_{i < j} J_{ij} \underline{m}_i \cdot \underline{m}_j + \sum E_i(\underline{m}_i)$

fit poly by sampling

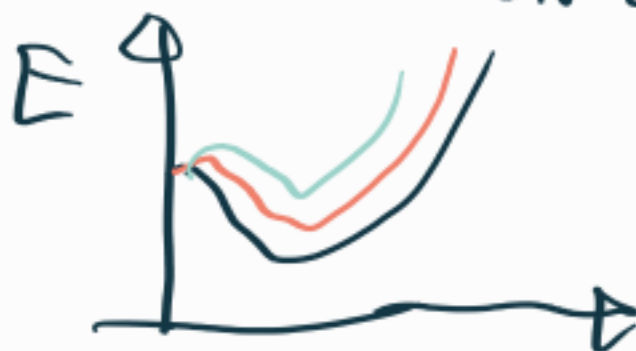
4th order poly

LSF energy landscape

approx

(all for Earth core sim.)

d) ML: LSF en landsc \sim local atomic env of spins



Size magn moment

using CBF + KRR

$$\left[\text{voronoi vol}_i, \tau_i, \theta_i, \phi_i, \dots, \sum_{n=1}^N \frac{e_i \cdot e_n}{r_{in}} \right]$$



$$E_i(m_i) = (a_i m_i^2 + b_i m_i^4)$$

~~2 different~~ models for the params
separate

Application:
Ab initio spin dynamics workflow
ASD-ALMD v. LLG
(ind. position updates)

B5.37 Unifying atom-centered descriptions and message passing machine learning schemes (Jigyasa Nigam, S. Pozdnyakov, G. Fraux, M. Ceriotti)

-) Recap ^{symmetrization} trans invar
-) Body-order hierarchy & rot sym
(scale invar \rightarrow 6LV MLST?)

\rightarrow Nigam ACDC Framework
 $|p_i\rangle$ vs $|\mu\rangle$

\rightarrow Nigam 2022 N-center framework
graph view MP-ACDC

Schütt 17, 18 Gilmer 17 Battla 18

Connects mp w. $|p_i\rangle$
 \rightarrow Tree of NV's
(invar equiv)

also
Battalio 2022

•) Example: MPNN doesn't in
github:

hcenter-reps
librasca/
equistore

Q&A

•) Johannes, UHalle

Q: ~~Q~~NNs: complete (WL test) did some?
A:

•) Q: nonlocality? ~~Q~~NNs^{MP}
A:

B5.18 Atomic cluster expansion for accurate and transferable interatomic potentials (Ralf Drautz)

- relation to others
- implicit Codis
- PACE, pyiron calphy, ~~AFISNAP~~ family
It's faster than others!
- Examples
- Charge transfer & magnetism
→ Drautz 2020 → **EMTapi**
spindynamics
- MPNN + ACE, mACE, MACE
Bockharel 2022 charge
- ^{Exp. t.} Antisym functions → ϵ_j → el struc calc
fast & acc TB via Hahn parameters

⑤ (Kernadilly)
talk
[B5.10, B5.32, B5.52, C1.13 posters
•) Q44
•)

Materials Virtual Lab

i) Multi-fidelity graph network GNN
for ~~DFT~~ ML Property mappings
(MEGNet)

ii) (also uses BO ~~in~~ for feature optimization)

iii) actually include, ^{validation} against exp. synthesis

iv) MLP limitations: $|Z|^2$ scaling

↓ mBody (actually, $|Z|^2$...)

↓ m3GNet

Tray
Data for entire PTE

How?

of mat
... which are
in the
mat Project

ArXiv 2022

"Universal MLP"

MAE ≤ 33 meV/atom

c) ~~LA~~ New AI-based DB:
matterverse.ai
31e6 \rightarrow 1e9 structures (goal)
(only few DFAs included)

Q & A

• A Origenov

Q: How incl all possible at envs?

A: only those in MP. ^{some are} sparse.

Q: checked if ~~at~~ envs not included?
No,

B5.20 Electronic structure properties from an atom-centered learning model of the electron density (Andrea Grisafi, A.M. Lewis, M. Rossi, M. Ceriotti)

- o) Prev Work:
 - o) Brockherde 177 $\text{Pot} \rightarrow \dots \rightarrow \text{Dens}$
 \hookrightarrow transf
 - o) Alred Compos. 166 2018 } grid
Jorgensen Bhowmik 2021 } based
 \hookrightarrow integrability
 - o) Ours: eldens in SH basis "middle way"
Grisafi 2018
 \hookrightarrow Res of Jd
- o) χ -SOAP; \hookrightarrow can't regress already
all coeffs coupled by ~~re~~ overlap mat
 \rightarrow expensive

o) transferable, linear ✓ 2018, molecules

•) Application:

$$n_e^{\text{DFT}} \xrightarrow{\text{ML}} n_e^{\text{ML}}(\underline{r}) \xrightarrow{\text{DFT}} E_{\text{xc}}[n_e^{\text{ML}}]$$

↳ indirect learning & direct learning
✓ direct learning

•) 2021 condensed phase: ice

✓ indirect learning (transferred well)

$$n_e^{\text{DFT}}(\underline{r}) \xrightarrow{\text{ML}} H^{\text{KS}}[n_e^{\text{ML}}(\underline{r})] \xrightarrow{\text{diag.}} \{\psi_k^{\text{KS}}(\underline{r}), \epsilon_k^{\text{KS}}\}$$


2022, Brisati

$$E_{\text{tot}}[n_e^{\text{ML}}]$$

Code: SALTED

Q & A

- *) Q: transfer to hybrid Ftal for HF exchange?
- A: No only PBE should try that.

•)  Situation not good
Be careful

•) How could get things really wrong?

Example: Covid lung image ~~data~~ diagnosis %
None was successful.

Why? Training data was
useless.

a) Data:

o) All ^{newly} DFT-PBE.

o) Data sources teach models their errors

o) Lo can use that to learn corrections systematic biases

o) our methods right now don't reflect on correl on training choices like train / test-split

o) Models

o) Architecture

o) Look up "information flow"

o) Design heavy reusable blocks in mind

o) ^{upgrade} multi-task / - fidelity / learn corrections

o) Transfer learning fine-tune, export, compose

Q&A

o) Q on reps

A: look up "periodic point clouds"
for crystal structure rep.

B5.51 Many-body Bayesian force field and uncertainty-aware MD from Bayesian active learning: Phase Transformations & Thermal Transport in SiC (Yu Xie, ..., B. Kozinsky)

•) FLARE = Mb Bayesian FF (MLP)
incl. "active learning" (BAL)

•) ACE + sparse GPR (SGPR)

•) BAL because MD data too small sample
pipeline of phase space ($\sim 10^3$)

Vandermaesen 2020

•) GPR: ^{reduce to} constant scaling w. training set size
via specific kernel choice Vandermaesen
2022 arXiv

•) GPU scaling to 27k devices via Kokkos Lib
(whole Oak Ridge supercomp)
($1e12$ atoms)

•) uncertainty-aware simulation
↳ out of distr. sampling during MD → training
↳ hierarchical training Xie 2021

o) Next:

- Feature reduction
- MPJ para

Q&A

o) GP scaling (MCEr)

Q: sparse GPR: ϵ is inv to training set size
No? No one does Full GP.

A: We noticed that it does scale.

o) BAL

Q: How does stability dep on GP kernel?
Sampling may be totally different.

A: We tested RBF, LPK diff powers,
• Found some diff in acc but
not sampling space.

-) GAP, extendable to other codes
-) AIMD in $\mathcal{O}(N^3)$, structures highly correlated
-) Sol: on-the-fly ML + AIMD
(throw away & build new if needed)
-) decision-making code extensible,
ships with GAP now, Python.
active data generation optional

CASUS Dresden

Fiedler2022 Review

•) What to learn?

$n(\epsilon)$? Problem for KE ~~file~~ entropy

So choose LDOS as target

can get $n(\epsilon)$ from it

...

•) MALA package (QE, PyTorch)
mala-project ELLI21 SNAP
Fiedler22 ϕ

•) $< 10 \text{ meV/atom}$

grid based
desc

•) HypOpt: Fiedler22 Speedup &
Automation \sim orders of mag

TODO look at this (Q&A below)

•) Applications:

of melting Al, 256 atoms

↳ LLOS \rightarrow $m(\tau)$ MAE

\downarrow
 E_{tot}

•) Interpolate btw params:

~~the~~ $T, p, \#N_{\text{atoms}}$

\downarrow
possible cause trained
on grid points, models
doesn't know about

\swarrow $\#N$

•) Sneak peek: > 100k atoms

linearly scaling at DFT acc.

*) Q&A

*) Hyp Opt?

A: See preprint

"Netw Arch Search wo. Training"

Thursday

Topological properties in real and momentum space C8b

Magnetic Skyrmions – Scientific fascination through ab initio theory

Stefan Blügel

-) New HEs Chiral ... Bouatzis 21
-) G Boumanoff 2018 → Reservoir Comp
materials realization in thin films
-) combinatorial problem of stacking
-) multiscale micromagnetic models
Atomic spin models

$$E_{(q, \hat{e}_{rot})}^{DFT} = E_{no SOC}^{DFT}(q) + \Delta E_{SOC}^{DFT}(q, \hat{e}_{rot}) \left| \begin{array}{l} J_{ij} \\ D_{ij} \\ \text{Lindhard} \\ \dots \end{array} \right.$$

-) Hensler 2022 Kavacik

→ J_{ij} DFT → ... → Hensler alloys

•)

matcloud & work now has
optimade BUG playground queries

optimade.science now has
an aggregator = queries ^{ALL} DBs at once
NLP: try
AI O quaternary

C3.51 Spin and orbital transport in rare earth
dichalcogenides: The case of EuS_2 (Mahmoud Zeer, ...,
Stefan Blügel, Yuriy Mokrousov)

→ Elast-O-Mat

→ Y.-G. Choi: Fry for SHE, OTE

→ What about 4P mats?

high magnon, bc f-els, strong SOC,
magnetic anisotropy

→ Workflow: FLEW → MLWF → Kubo formula
CPA+U Wannier90 Spin/orbit card

System: EuS_2

Q&A

Posters

Poster B5.10 Efficient parameterization of the atomic cluster expansion

Bochkarev, Drautz

ACE \rightarrow PACE Lumps

Q: 1) only energy & forces or general?
2)

Poster B5.32 Active learning strategies for atomic cluster expansion (ACE) model

Lysogorskiy, Drautz

ACE "slightly" non-linear
active learning: ensemble learning vs. (multiple)
D-optimality (maxVol) (single)

Podryabinkin 2017

Y. Zhang 2020

Poster B5.31 Extending Atomic Cluster Expansion to
Equivariance, Many Elements and Long-range
Kovacs, Csanyi

MACE, Multi-ACE, GNN.

Allegro does things on edges
we on nodes ^{better} + efficiency

Multi-ACE: able to handle many-elmt datasets

Tensor-reduced ACE

10x less basis fns cmp. to Nequ3P
needed for same accuracy

Tensor Products over nodes instead of edges
(Nequ3P)

Poster B10.02 DFTK: A multidisciplinary Julia toolkit for electronic structure simulations
Michael Herbst, Cances

Pay attention to VFTK ongoing development!

Building Full Julia toolchain

$\text{DFTK} \rightarrow \dots \rightarrow \text{MD}$ preconditioning
 (underlined) UQ across the scale

up coming:

d) ML - solid-state XC models

Poster B5.17 Compressing local atom neighbourhood densities James P. Darby (1), James R. Kermode (1), Gábor Csányi (2)

Same as in the paper

Goal: $|Z| = 25$ elmts, different compositions

•) DG: \rightarrow PTE \rightarrow 3d transition metals d-block
 \rightarrow generated 3 to 25 random elms ^{beyond} fcc/bcc
 \rightarrow 25K most different system
uniform distr.

•) Rep SOAP $|Z|^2$ scaling \downarrow
 \rightarrow Willatt 2018 project PTE \rightarrow 2D space
So Nataliya applied this here
"pseudospices"

Implemented
anywhere?

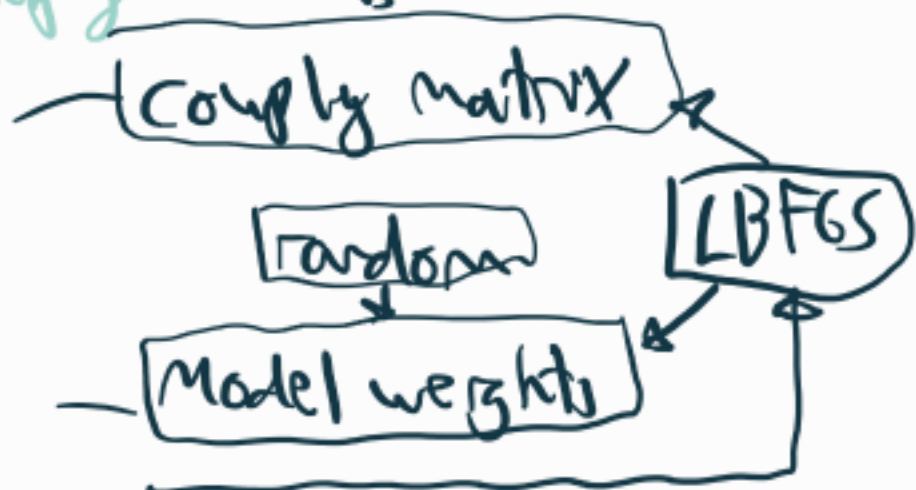
Problem: makes it, becomes
non-linear, becomes 2-step
optimization problem

2) Answer: They implemented it in PyTorch.

Model

$$SE = SE^{int} \times \text{couple matrix} \downarrow$$

:



0) Test : Linear \times pseudo chrt, nonlin model
 $\rightarrow 13 \text{ meV/at}$

Pure extrapolation: MProject, $E_{\text{formation}}$
of all binaries

MD Au-Cu / MLP

MD sim 6 compo HE alloy ~~p~~ / MLP

Q&A

-) Point of HEalboys is to maximize entropy not free energy
-)

•) TODO look at implmtn

Natalya: Implm on github
contact in case

Poster B5.75 Kernel Charge Equilibration: Learning Charge
Distributions in Materials and Molecules
Martin Vondrák

B5.75 Vondrák FHI

KQEq Code on GitLab

for long-range interactions
charge equilibration

from env-dep electronegativity

via Kernel Charge Equilibration

B5.45 Equivariant neural networks as a natural and dataefficient method for machine learning many-body prop.
(Martin Uhrin, A. Zadoks, L. Binci, N. Marzari, I. Timrov)

.) For Hubbard corrections

o) Normally $|A_i, \lambda, \mu\rangle \rightarrow$ target
Here instead el. str. props \rightarrow

.) Motivation: transition metals (poor xc)
 \rightarrow Hub cor to DFT \approx in SCF
 $E_{\text{DFT}} + U + V = E_{\text{DFT}} + E_{U+V}$
for hybridized states

Timrov 2018, 2022 from DFPT

.) SCF with U_{in}, V_{in} initial guess

extra-SCF for U, V

on-site term hopping term
species that pair
 $n_{1,d}$ and $n_{2,d}$

TRIP invar

occup matrices $n_{mm'}$ are $SO(3)$

→ e3nn lib, tensor decomp

permutation of spin labels $\uparrow \downarrow$

→ perm invar polys Hadamard prod

U :

6) model: in → \otimes → nonlin → \otimes → U_{out}

V : $\otimes \rightarrow$

•) Data: battery materials
Training: the usual

•) compare SCF & ML- U / converge
same w. V

•) Bias check: just trained on iteration
Zero: passed (learns V_{new} response)

→ Transferability: $U \checkmark, V \nless$

✓

↳ Future: AiiDA automated workflow ML

TODO: contact Muhrin!

Talked w. Francisco from AiiDA Team about my use case and AiiDA-ML plans, took my contacts.

Q&A

Spontaneous and externally driven quantum spinfluctuations
at the nanoscale

Samir Lounis

-) They used juk~~K~~R & KKRimp
-) see abstract
-) $\text{KKR}_{\text{SUSC}} = \text{TD DFT} + \text{SOC}$
for adatoms out χ
-) New state: spin atom, Bowatz 2020
Kondo effect example is not Kondo^{from} effect
meV energy scale

•) Very different from what you'd expect

•) q spin fluctuations:

$\times c_s$
DFT predicts large anisotropy

wrong, how to resolve ~~that~~

predicting magnetic instabilities

(motivation: memory device ^{miniaturization} storage)

\leftarrow ^{can} correction term

•) Lounis' "Drosophila system"
atoms on silver

•) ^{how to} reduce $ispfluc$: 1)...
2)...

•) 2020 extract J_{ij} \underline{D}_{ij} ^{TBBFT} incl 0 point $spfluct$.

they tend to reduce J_{ij} in \underline{D}_{ij}

TOVO @rness: implications
topological magnetism?

∞) Did this to revisit 2010, 12
work Lowrie discrepancy to
experiments.
w. Fluctuations 2020 better agreement

•) Summary
o) Brinker 2022
o) ...

Q&A

•) small flux scale, what if DFT+U?
Yes, calc were LDA. ...

B5.07 A pre-training augmented deep learning framework to predict the materials prop. (K. Das, B. Samanta, P. Goyal, S.-C. Lee, Satadeep Bhattacharjee, N. Ganguly)

a) Crystal graph GCNN paper
Grossmann

b) → multi-graph colored ^{try that} ^{TO DO}

c) autoencoder: Crys AE ^{to overcome small data for DL w. SSL}

predictor: Crys X PP | paper hpj
w. feature selector

d) / for
XAJ
~~with~~ LASSO

graph embedding | predictor
GCNN | MLP

e) Comparison. GCNN
MIT GCNN
MEONET
ELEMNET
CRYSEXPP

•) Removes "DFT bias"
via exp. data finetuning

•) XAJ w. Feature Selector

•) Summary

•) Q&A

Q: Size of latent space?

A: $64 \times < \text{input space}$

Poster B5.63 Jacobi-Legendre potentials

Michelangelo Domina, Matteo Cobelli and Stefano Sanvito

This is used also in B5.19 and C3.55,
among others.

Poster C3.55 A spectral-neighbour representation for vector fields: machine-learning potentials including spin

Michelangelo Domina, Matteo Cobelli, Stefano Sanvito

From SSanvito twitter Aug 24: "[...] a new machine learning potential for magnetism"

- a) Insight $E = \sum E_i$ often as
Taylor expansion from
body-ordered rep (if
write out)
- b) "Most notable in recent years"
ACE \hookrightarrow not as accurate
Nequip \hookrightarrow slower
- c) \rightarrow MACE $\checkmark \checkmark$ MPNN
- d) Insight: $\text{range}^{(6)} = \# \text{ layers}$
- e) MPNNs have 3 phases
 - 1) message constr
 - 2) update
 - 3) readout

o) Limitations of MPNNs now:

2-body messages: incomplete

layers = expressivity

N -body expressive

→ MACE

o) 1) MCo: TaySE of NNs
idea: complete basis inspired by ACE

\prod tensor prod only on nodes

better prefactor not on edges
like NequIP

Saves computation

Messy as linear comb of compl basis

o) ^{Proof:} → can red #Lay to 2, still better

o) Power Law Training Size

Better For Higher-Order

-) ~~then~~ MACE 5-10x faster
-) Trained on 300K+ benchmark

•) Unified context of ML Potentials:

Multi-ACE.

SOAP, MACE, ACE, NequIP all
prints in there, MACE currently best

•) Code: github ACE-suite mace

Q&A

•) Krossi group

Q: No I didn't understand

•) Cost is constant with # species
since embedding
have no scaling w. that

! todo got to go MPNN!

B5.30 ML modeling of potential-energy surf. and mol.
property prediction with a 2-kernel approach: resolving the
multiscale challenge (Artem Kokorin, ..., A. Tkatchenko)

*) Limitation of single-kernel
approaches: different curvatures of
PES, multiscale PES



→ 2-kernel lincomb

*) as matrix not: $\underline{Z} = \underline{A} \underline{a} + \underline{B} \underline{b}$

→ multiscale

*) Test: error valued for MD17
kernels $\hat{\Gamma}^1, e^{-F}$ in small data regime

2) Test on QM7-X (TZK 6)

El Desc VFTB ^{an} ~~an~~-VFTB #CBFV
Geo Desc Bob #SBFV (small) ⁶⁰⁰
SLATM #SBFV (large)
→ Combine single kernel 2ck

OR

→ Use double-kernel 2kernel
(use 2 feat spaces)

Result: slightly better MAE ^{~10} En ^{~600}

Take home msg: ~~El Desc~~ Geo Desc Bob 2kernel
better than SLATM 1kernel
→ ~20k

Q&A

• Q: multibcd?

See also poster C1.25!
TDW (spin-dep potential)

•) DG: Random strucs
 Grid based JL exp of eldens
 Exp in basis
 LinReg
 Starting guess for DFT
 ind

•) Exp = 2 body + 3 body terms + ...
 \sqrt{ij} $\sqrt{ij}\sqrt{ij} < ij$

$\psi(\underline{r}) = \sum_{\text{in Jacobi}} + \sum_{\text{Leg polys smooth to 0}}$

5) App: Benzene

DG: 30 snapshots MD, Brock 2017

→ VASP → 180^3 grid

→ Hypo 6P,

Lin Exp fsize 1554

Grid sampling ~ eldins + uniform
< 1% of data set Random sample

5) Results: plot diff

MAE 0.003 e/ \AA^3

6) Al $N_{\text{tr}}=10, N_{\text{test}}=10$ MD

MoS₂ 1H 1T phases → pred on π phases

fsize 2800

-) ~~Start~~ As starting guess ^{ES eqn}
 5 non SCF steps block Davidson iter sol
 comp w. $E_{GS} : E_0 - E_{NSCF}$
 ~ 60 vs 1
 Force
~~Set~~

-) Scaling
 small $\Delta E \rightarrow$ small ΔE ✓

-) Summary

-) Linmodel ✓

-) As acc as to fields 1-5 mV

-) Extrapol

-) Speed up,

scales to multi-species
 systems **TOPO**

•) JL exp: poster B5.63
also on arXiv

Q&A

-) Benchmark model carefully
not just MAE, RMSE, also density
-) Also tried LDA, hybrid functionals, ...
-) Looking into wf now

- a) UK HPC Dec21 use
1/3 DFT/MD 40% +
(30% VASP alone)
- b) AIMD: $\Psi, g(\underline{r})$ is thrown away
Why not do that?
- c) Q_e $\xrightarrow{1e6}$ density $\xrightarrow{1e6 - \text{length/time/calc}}$ FF
WF
- d) "Short range QM region is solved ^{*}2020"
* exchang imprint
- e) Hermitian imprint GAP-RSS
Does it converge? It does

o) The Key is rep: TRIP invariance
locality
completeness

o) BPNN 2007 quad scaling
Density Trick 2010-2013 (power spec
base spec SOAP)

Later realized corresp to each other
power spec Basis exp of RDF, ADF

o) Added Kernel fitting (GPR 2021)
w. Low Rank Approx of \underline{K} in reality

o) It works! 2014

o) key message 1: Sym Rep

o) Next try: General-Purpose MLP
for one material: Si 2018

o) Random Structure Search:

Only ML method gets BFT acc

o) Applications:

Renton IrO_2

Cerotti H_2 qg H

Derfger PCM on ~~same~~ -levelize-scale

BASE Csanxi Catalysis CO_2 hydrogenation



↳ convergence in iterative training needed

bad model $\xrightarrow{\text{data}}$ good model

o) Key Mes, #2

Iterative construction of fitting DB
is mandatory

— That was 2020

•) Dark funds:

o) Incompleteness of 3-body reps
Cerretti 2020
Parseit and Goedecker 2022

o) Solution: ACE

$$\text{SOAP: } p_{q'q} \sim c_{nlm} c_{n'l'm}$$

$$\text{bispectrum } b_1 b_2 b_3 \sim c_{n_1 l_1 m_1} c_{n_2 l_2 m_2} c_{n_3 l_3 m_3}$$

ACE: ; just continuous

New notation, efficient eval order

No need for kernels anymore
→ linear modeling

→ TQDD Really?

b) That was 2021. Then:

c) E(3)-E6NN Kozinsky 2021
was applicable to material Nequ3P
and 2x better than ACE

Why is it so good?
d) Design space of E(3) 2022
↳ Unify MPNN & ACE

ACE is passed around 1-atom
neither ACE nor GAP could this

MAE poster
// remember Multi-ACE

and generalize very well

e) ACE is smooth but wrong when
there is no data. Not Nequ3P.

•) Future:

•) "Short-range fitting ^{now really} is solved" ^{*}
* until proven wrong

•) inter/intra molec interact simply

•) LR interactions: flexible electrostatics,
charge transfer,

•) Full SCF of DFT but on atom
not cont $\rho(r)$

•) coarse grained models

b) Uncertainty quant

→ DFTK poster

c) Inverse problem: Prop → ^{Fitting} DB

d) New questions because
emp pots were not system convgt

e) Key message #3: Extrapolation is possible
ACE & MPNNs

- ↳ Marzari Closing Note
- ↳ 3 million fold increase
1992-2022 speed in
atomistic simulation