

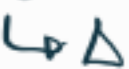

Tue

-) ME HydraGNN etc → collab, bawly ML-KKR
-) Masoumeh 2D semi-inf 7d → JLCDM
↳ collab, datasets ↳ see email gmail

Wed

-) Nihad CrTe₂ etc 2D magnet
QE → KKR → spirit
Get the data. $N = ?$ ← datasets, jiji-pred
General concern
-) Akash TCD
•) smeagol + JLCDM in future
↳ GF
↳ collab, ML-Dens
-) How did viz
x-z view crystal lattice
viz ↳ early slide
-) Abhis Gilbert damping in SKKR
↳ spin dynamics
↳ Slide dimers FM, AFM AgAuCu
↳ relevant for jiji-pred?
-) Belashchenko
•) Vector SH for SOT
↳ Representations spin
↳ Dataset Generation
-) cheap way to simulate disorder
with 10k atoms sim. not possible w. SCF
CPA, just shift the potential

o) Szemiyogh

o) SLESTA can by defg entities (in this case, An trianguleres  on surfaces), directly calc J_{ij} interaction btw those entities . See paper martinez 2023 PBLQ (or sth) model params.

J_{ij} -prediction,
model extension,
dataset generation

Also see next preprint
about SLESTA mag. interaction
implmtn.

o) Discussion SB: ^{How to treat} spin-1 system in DFT?

SB: spin-1 is $\text{spin}=\frac{1}{2} + \text{spin}=\frac{1}{2}$. Two els.
DFT is one-el. OP: this is microtheory, so
not DFT, so applicable. SB: No. Haldane was
quantum spin chain. After 40 years of
DFT need a sln to treat spin-1 systems.

o) PM Q: Always start w a sentence why he
valued the talk in online summary. ~~Nice~~ Then
pose question. Nice touch.

1) PMn^{3+} in my experience, calc adatoms on surfaces, always loses $\text{spin}^{-\frac{1}{2}}$ or spin^{-1} character. Some part lost " (did he say 'by spin flow into the bulk', or similar?). End up with $\text{spin}^{-1.2}$ or similar.

2) Posters

a) LMU group

b) KKR + CPA ϵ_{ij} ... effects on displacements (lattice distortions) in ternary compounds

$$(H = \sum_{ij} \epsilon_{ij}^{\alpha\beta} e_i^{\alpha} e_j^{\beta} (u_{ik} \dots + \dots))$$

Q: Is this relevant/possible w. JKKR, TJs?

c) Akash Bajaj

d) ∇ see above

e) Q: Accommodation Dublin

•) Marrazzo

•) Group 1 postdoc avail. NN ML/AP
+ AiDA
probably for quantum materials

Thursday

*) Sanderson

jij-prediction,
papers

•) (RMOZ: For QAHE, want large $|j_{ij}|$ for FM.

But FM kills SC (for TQC).

Found "unconventional AHE" in

non-collinear AFM materials (non-coll contributions besides $\uparrow\uparrow$ FM spin dirs induce AHE in this case).

Q&PR: Take into consideration in j_{ij} paper? (consider though, different material: _____)

•) (Also just interesting wrt magnetic impemp analysis, there were several such contrbs)

•) Hifalussy

Nice intro to MZMs. "Saw a lot of calc.ing j_{ij} 's in this workshop."

•) Aceves

•) TITAN-FZJ/TITAN

•) Diagrammatic way of showing j_{ij} 's.
Maybe adopt that

jij
prediction

•) Biermann

•) Philosophy: One can view Σ of DMFT like ρ of KS-DFT (rep = $a \times s \times s$) (not real sys)

•) Generalized cavity construction
↳ ~~is~~ is a generalization (MB, non-local) of KKR impurity embedding (single-particle, local) (Ayson eq) (or Anderson imp emb?)

•) Q: Bakshchenko: GCC sounds a lot like the "Onsager".

•) Minar novel
•) AJ for new ARPES or sth dichroism for TJs ^{get} orbital info (statis linear)
TRDAD Time Reversal Dichr in Angular ...
Circular dichroism + TRD for Berry curvature

•) HAXPES 2024 conference
AJ for electron spectroscopy