Magnetic properties from first principles simulations

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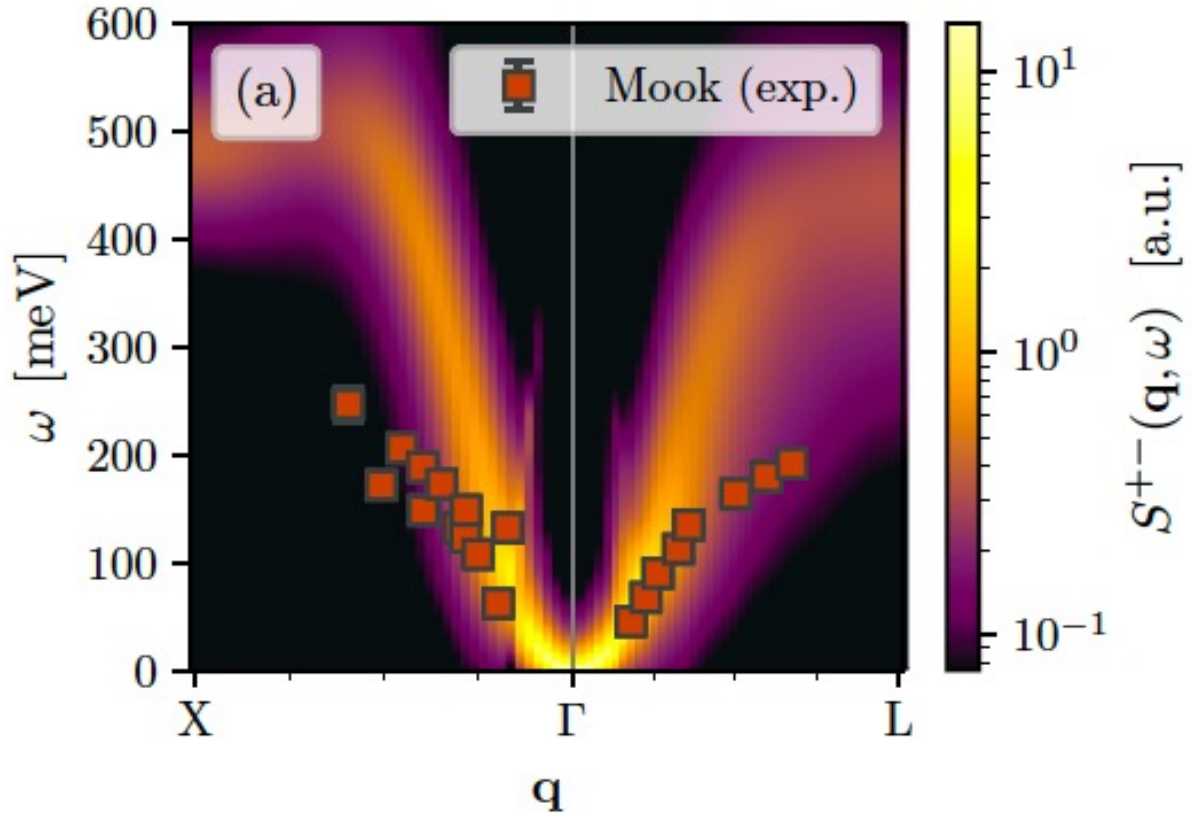
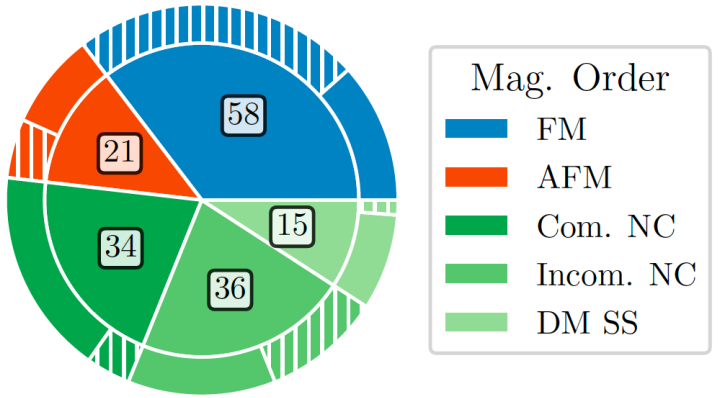
Department of Physics - Technical University of Denmark
DMSC workshop 5/10-2023

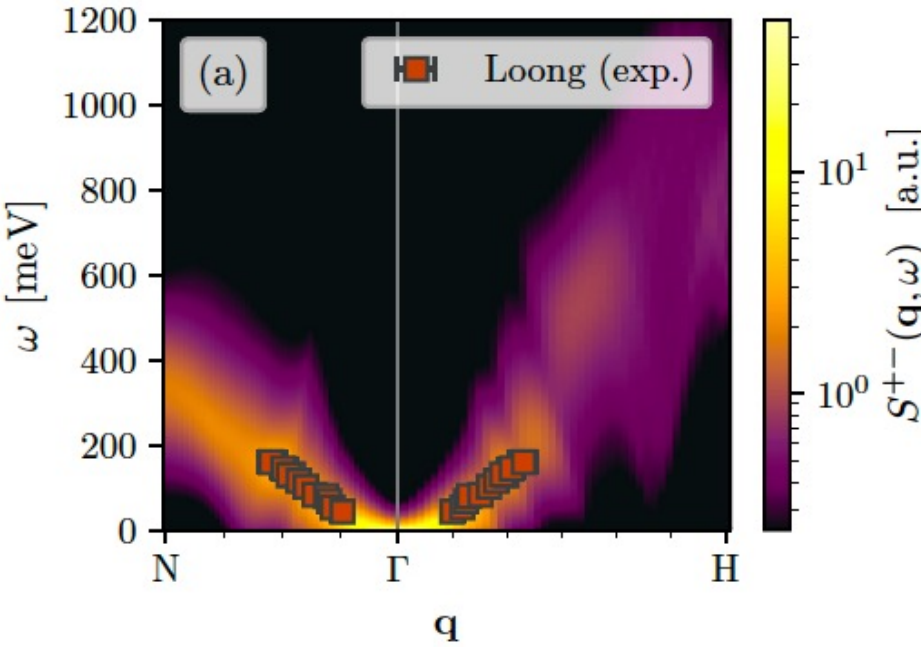


Outline

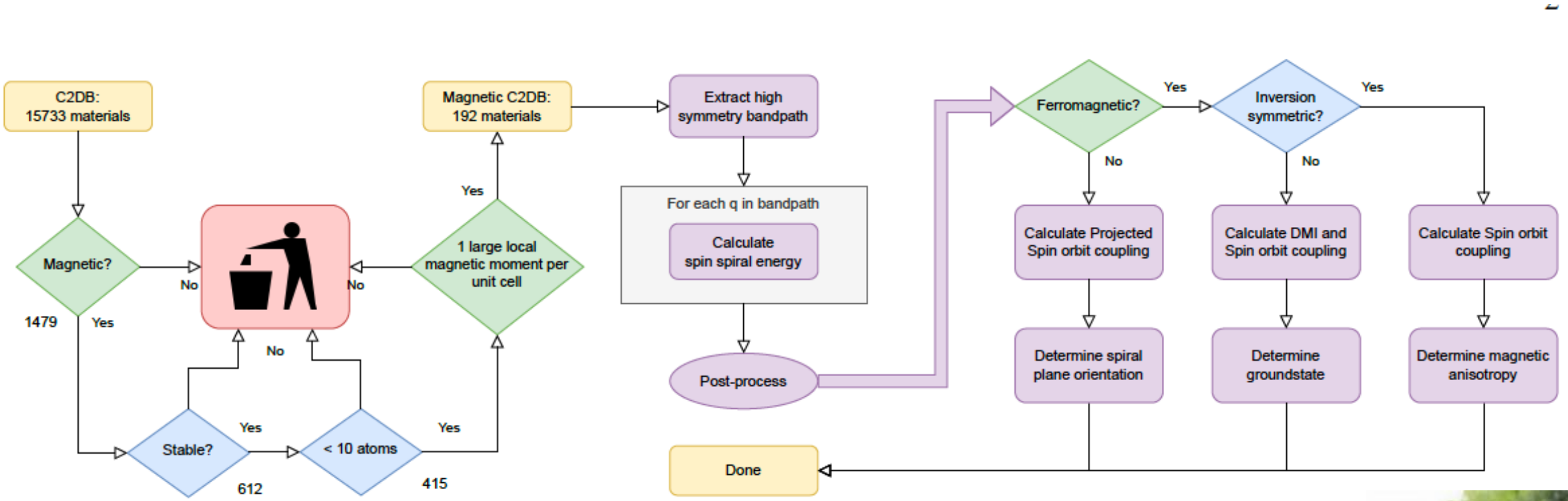
- Ground state magnetic order from high throughput computations



- Magnetic excitations from time-dependent density functional theory



High throughput calculations



192 2D magnetic materials from the C2DB

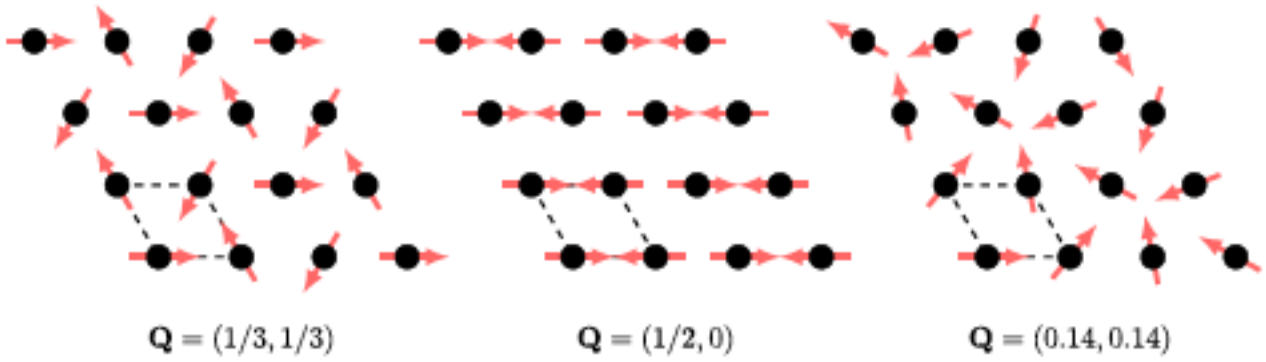
Ground states analyzed from spin spiral calculations

Calculations performed by Joachim Sødequist

J. Sødequist and T. Olsen, *arXiv:2309.11945*

Spin spirals

- Any single-q state can be calculated from the Generalized Bloch theorem



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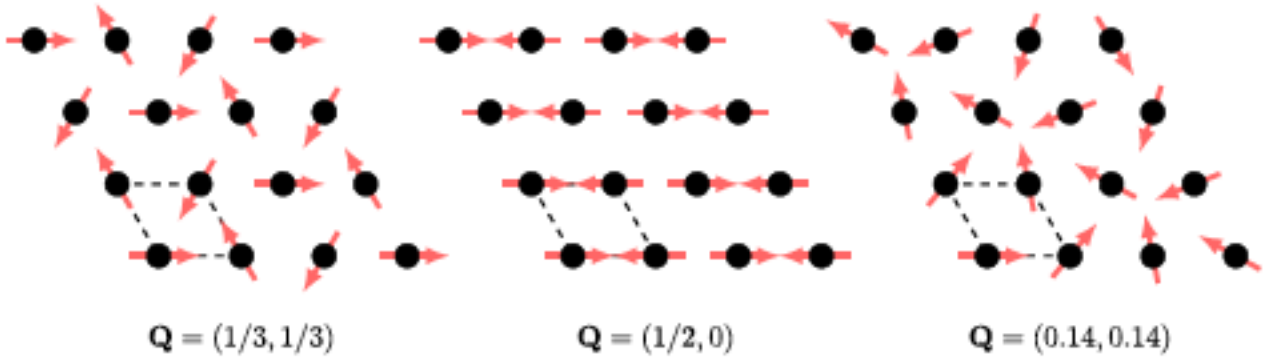

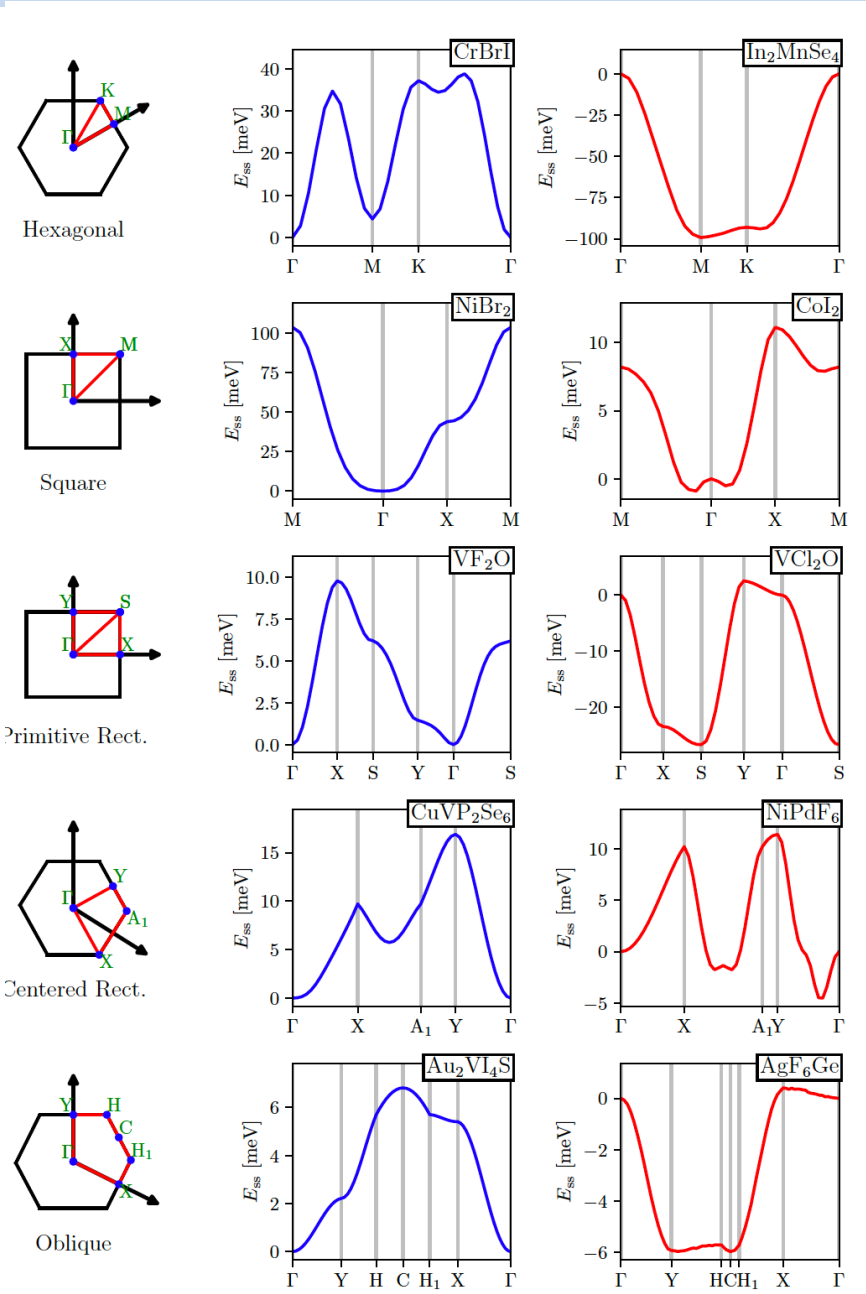

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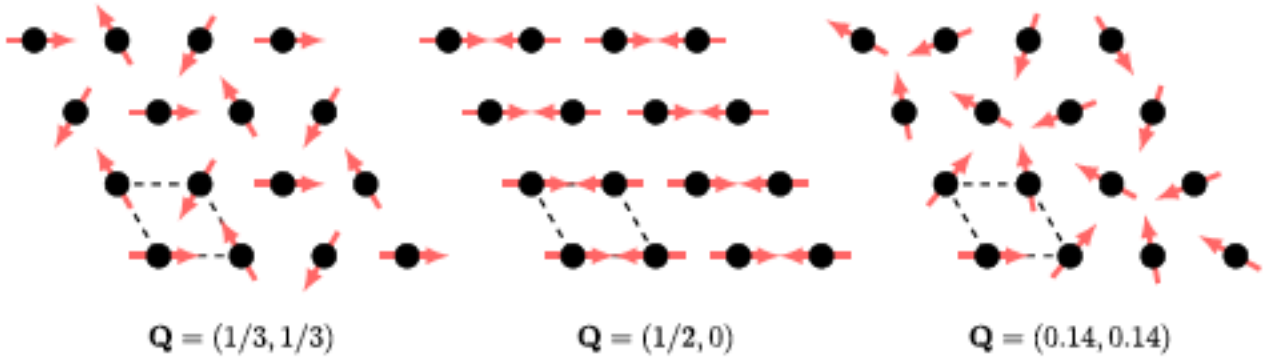
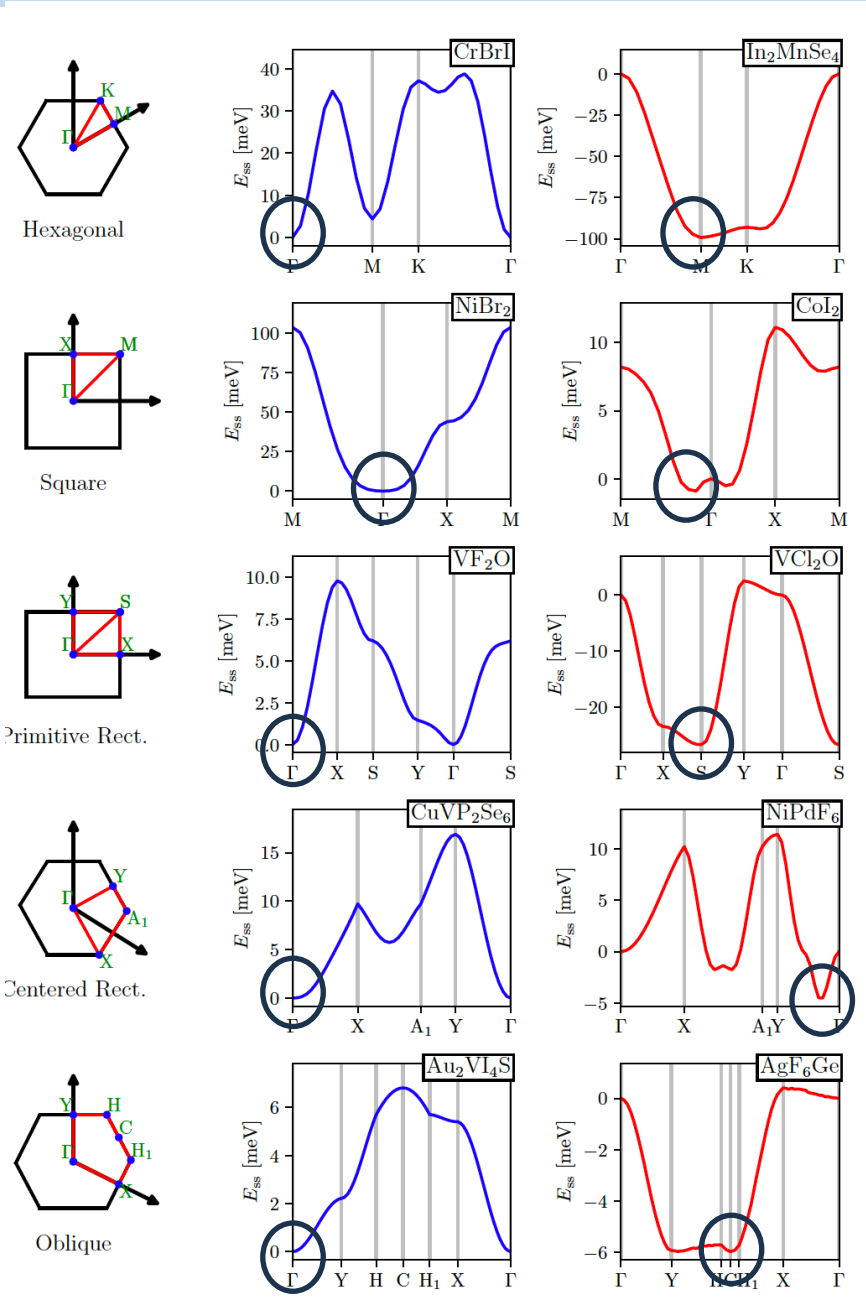


- The ground state is determined by the minimum energy



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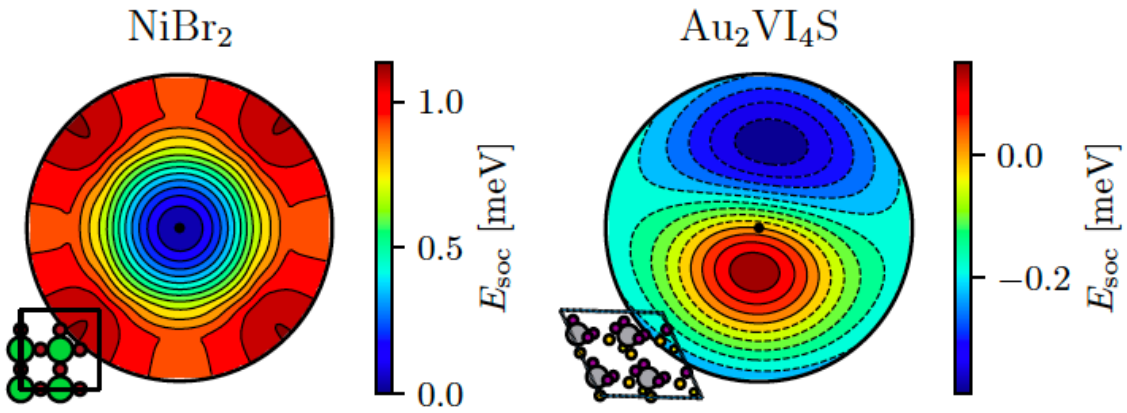
Magnetic anisotropy

- For collinear systems spin-orbit coupling is used to determine easy axis

- In-plane anisotropy signals higher order exchange interactions



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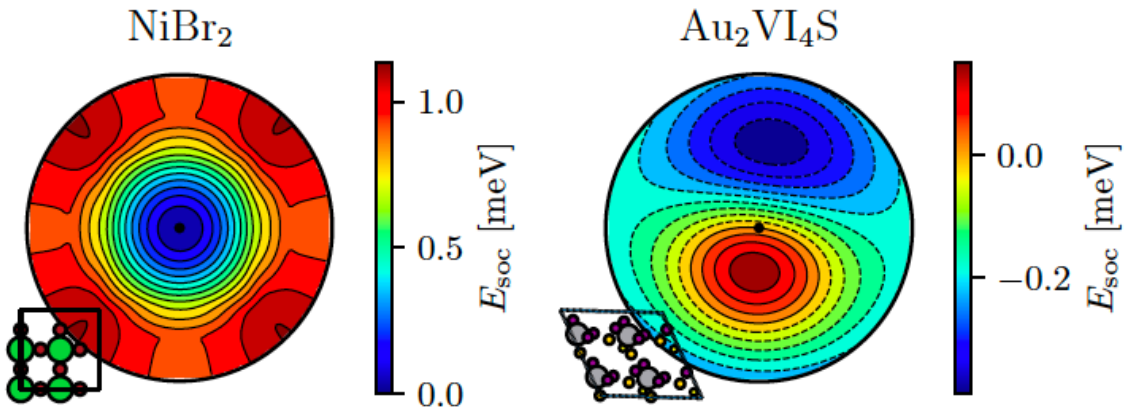
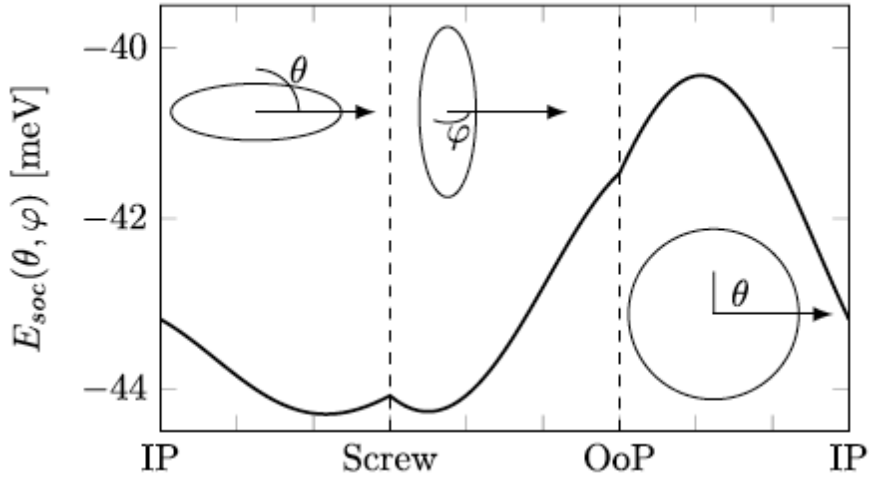
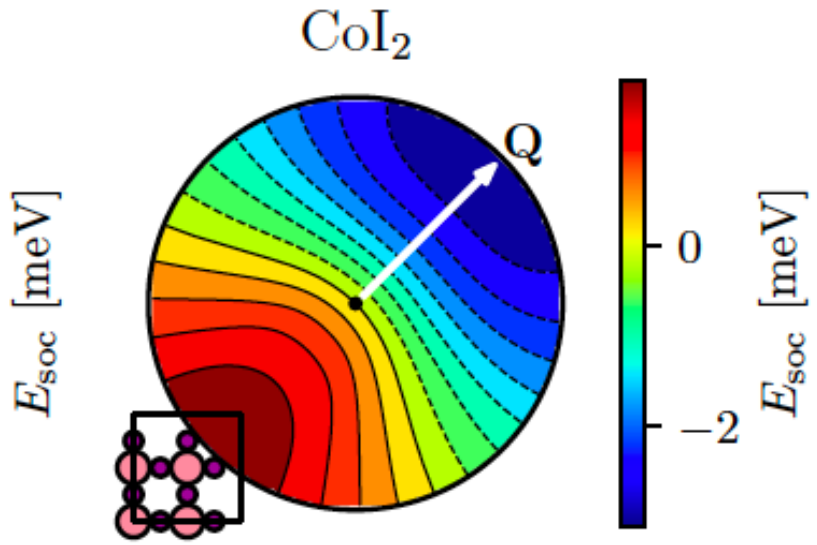


For spin spirals SOC is used to determine orientation of spiral plane





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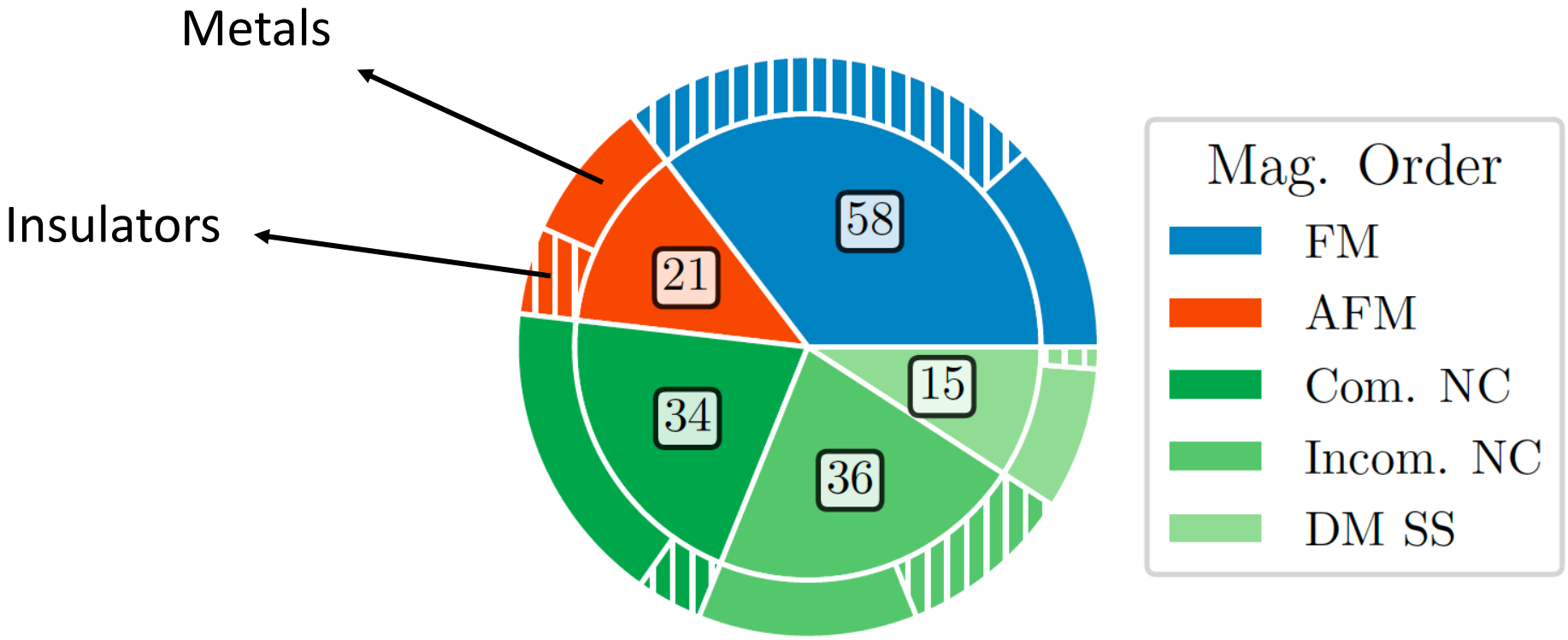
Summary of magnetic order in C2DB



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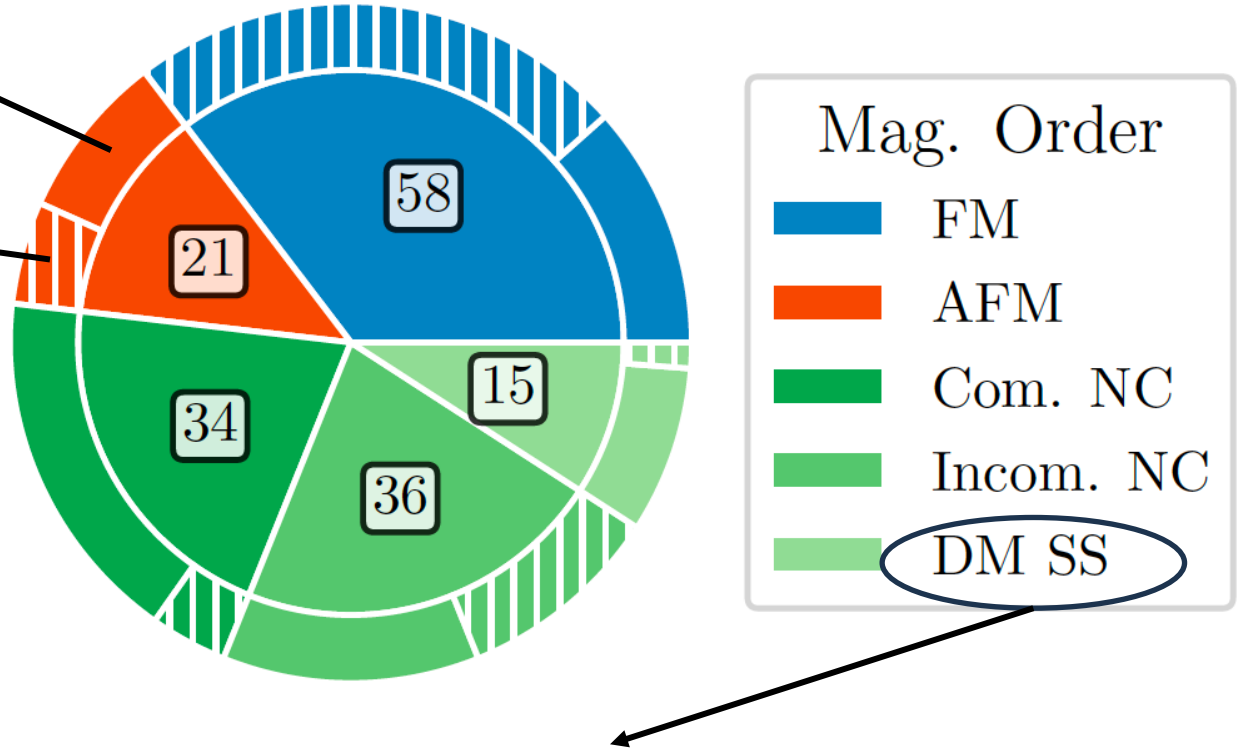
Summary of magnetic order in C2DB

Metals

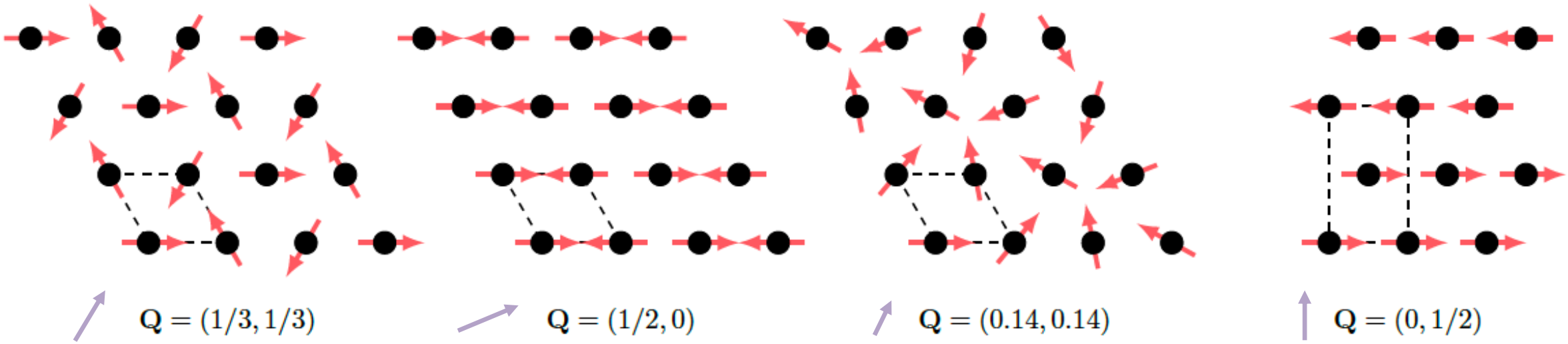
Insulators



Ferromagnets without inversion symmetry may destabilize into chiral spin spirals by Dzyaloshinskii-Moriya interactions

J. Sødequist and T. Olsen, *arXiv:2309.11945*

Type II multiferroics in experimentally known transition metal halides



$P \neq 0$ $P = 0$ $P \neq 0$ $P = 0$

J. Sødequist and T. Olsen, *2D Materials* **10** 035016 (2023)

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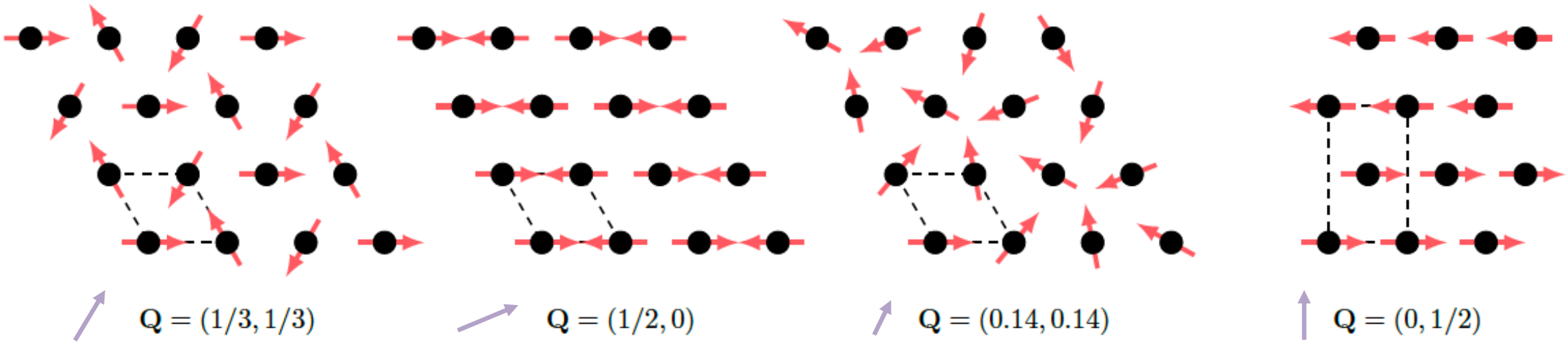

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$(q = 1/7,1/7)$

$(q = 1/3,1/3)$

	(θ, φ)	$P_{\parallel}$	$P_{\perp}$	P_z
VI_2	(11, 0)	-0.6 (-31)	290 (96)	0.05 (0.11)
$NiCl_2$	(90, -30)	-37 (-1.4)	76 (15)	3.5(-5.1)
$NiBr_2$	(69, -10)	12 (-6)	340 (32)	26 (37)
NiI_2	(70, 0)	-8 (-48)	1890 (400)	-0.18 (12)
$MnBr_2$	(90, 0)	430 (38)	0 (0.02)	0 (0)
MnI_2	(0, 0)	0 (0.6)	0.3 (-7)	-260 (-105)

fC/m

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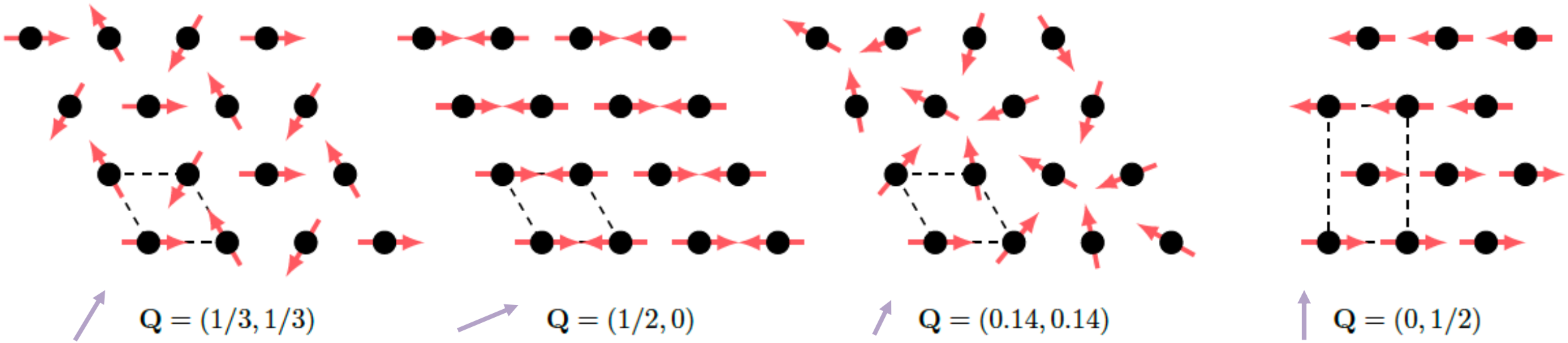

Proper screw

Failure of KNB model!

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Magnons from the Heisenberg-DFT approach

- DFT is usually good at total energy differences
- We can thus map out spin configurations to obtain Heisenberg parameters

$$H = -\frac{1}{2}\sum_{ij} J_{ij}^{ab} \boldsymbol{S}_i^a \cdot \boldsymbol{S}_j^b$$

- Magnon dispersion depends on $J^{ab}(\boldsymbol{q})$ which is extracted directly

F. Durhuus. T. Skovhus and T. Olsen, *J. Phys.: Cond. Mat.* **35** 105802 (2023)

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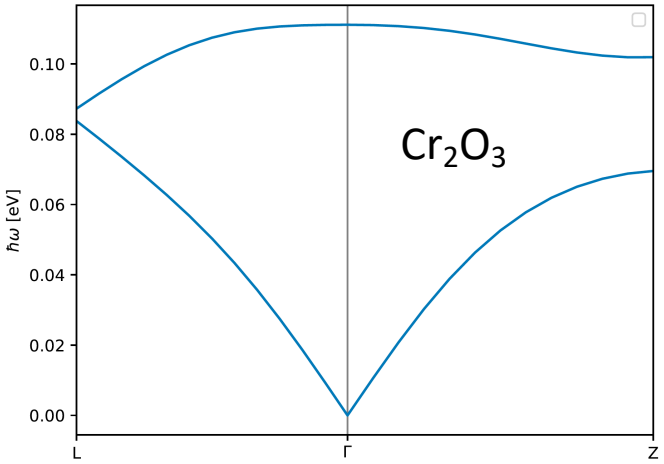

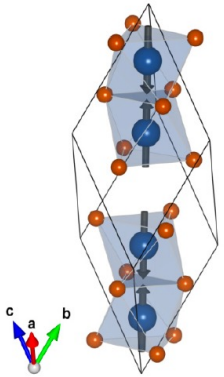

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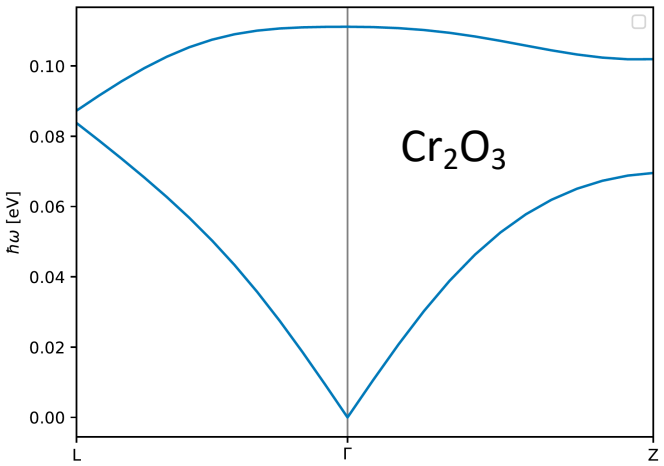

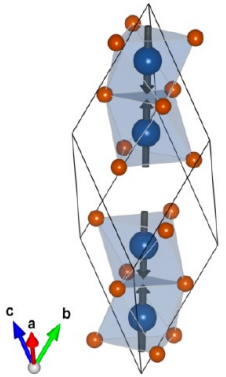

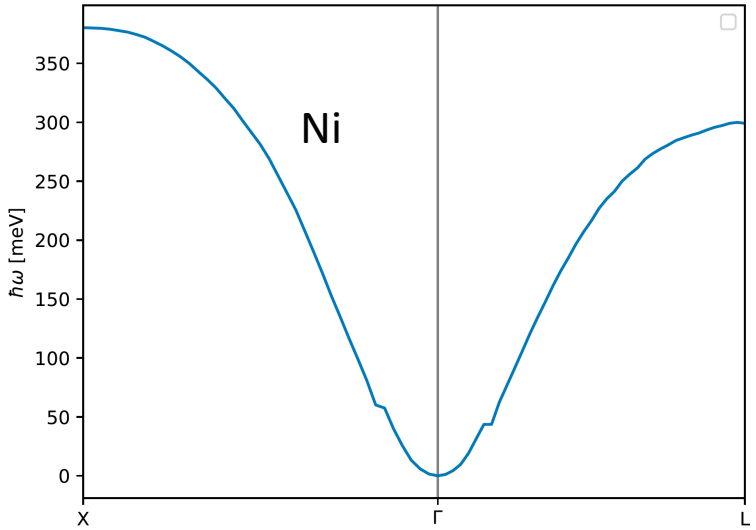

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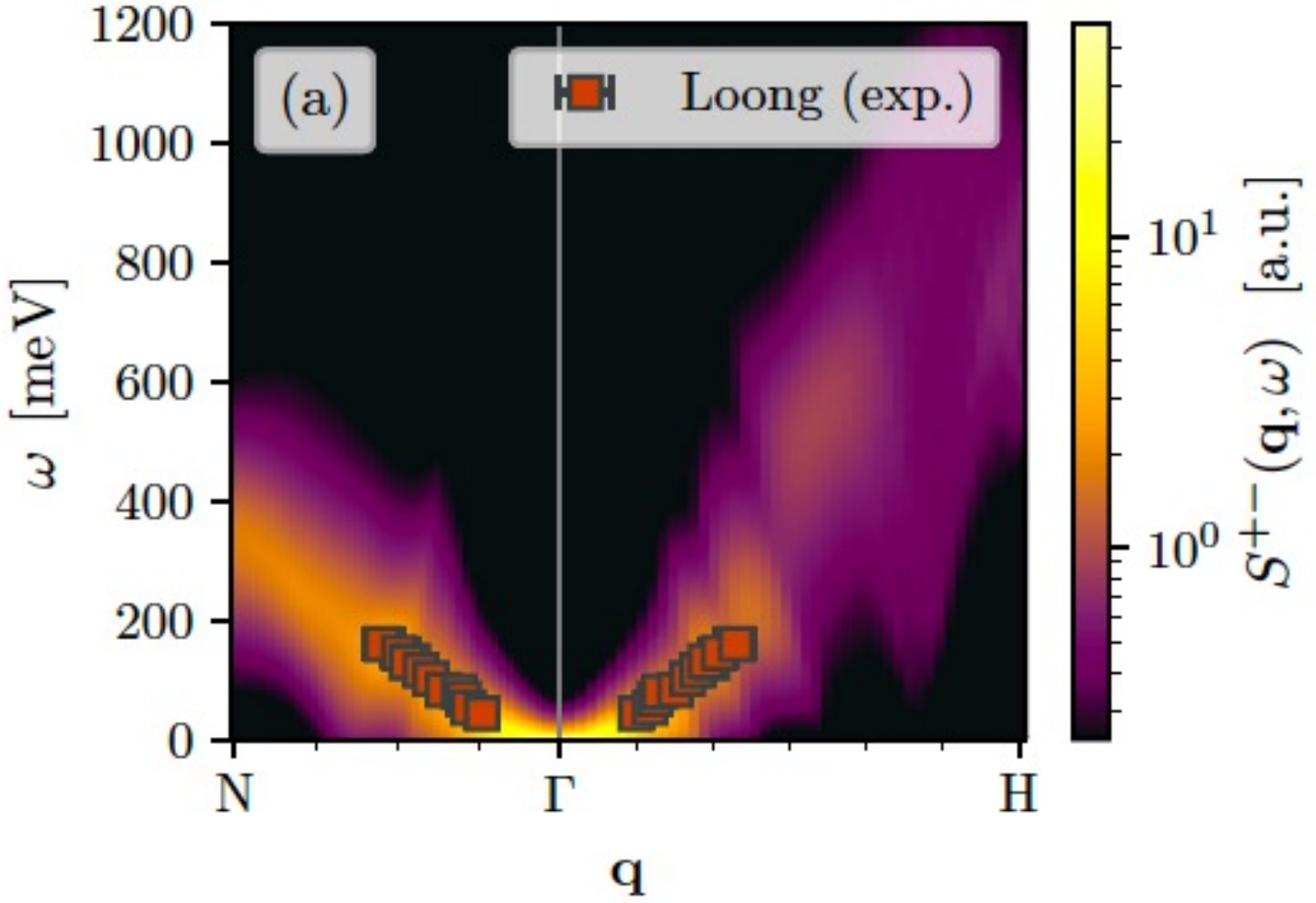
Magnetic excitations from TDDFT

The full interacting transverse susceptibilty can be obtained from TDDFT

bcc Fe

The associated spectral function yields the Landau damping as well as dispersion of magnons

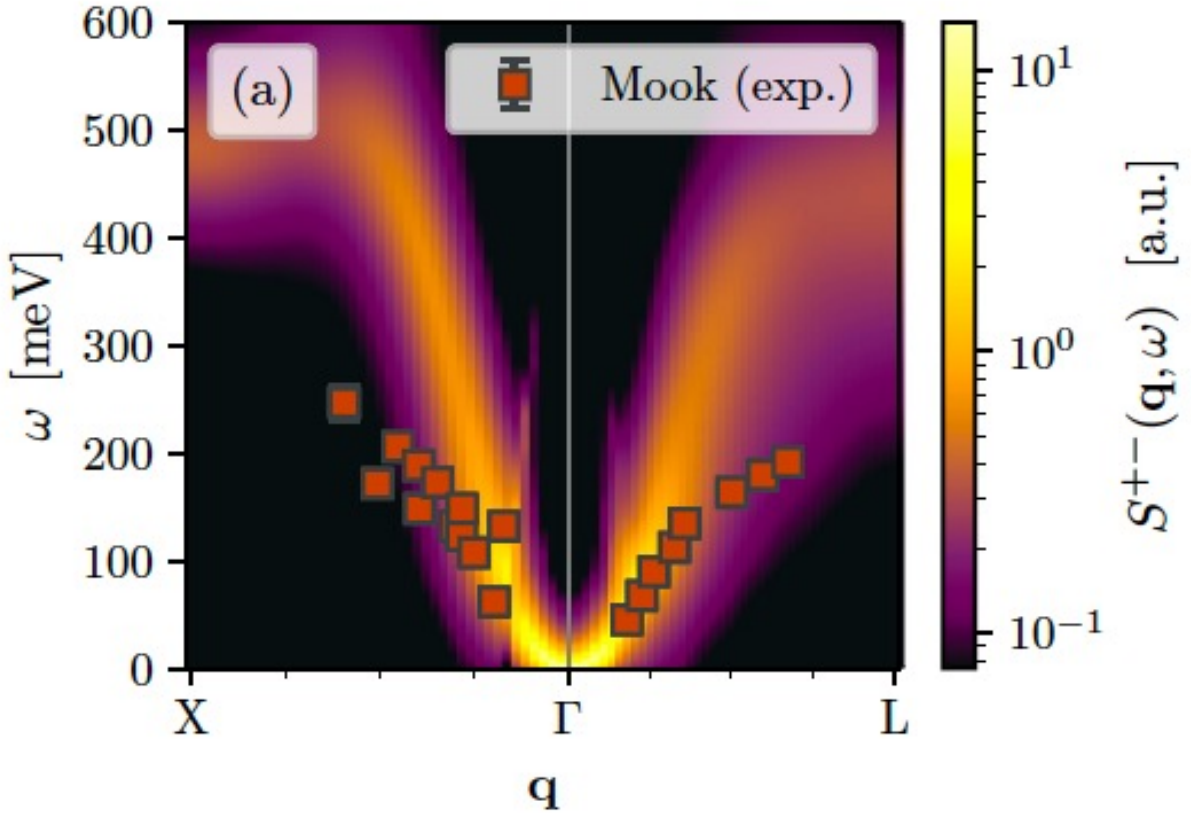
Calculations performed by Thorbjørn Skovhus

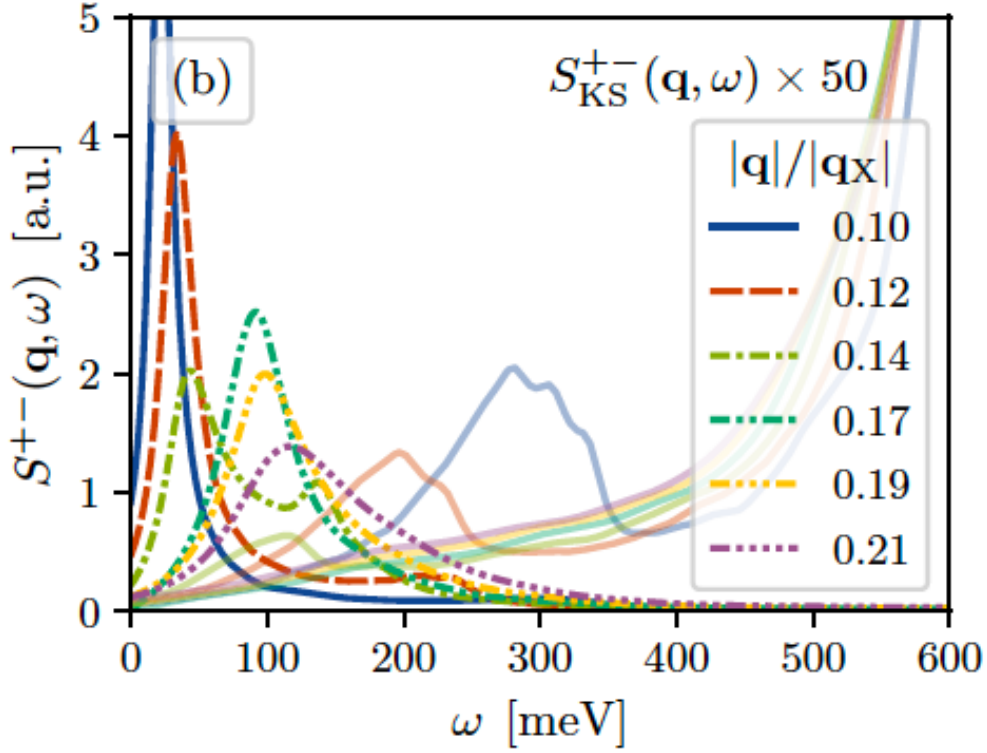


T. Skovhus and T. Olsen, *Phys. Rev. B* **103** 245110 (2021)

Magnetic excitations from TDDFT

fcc Ni





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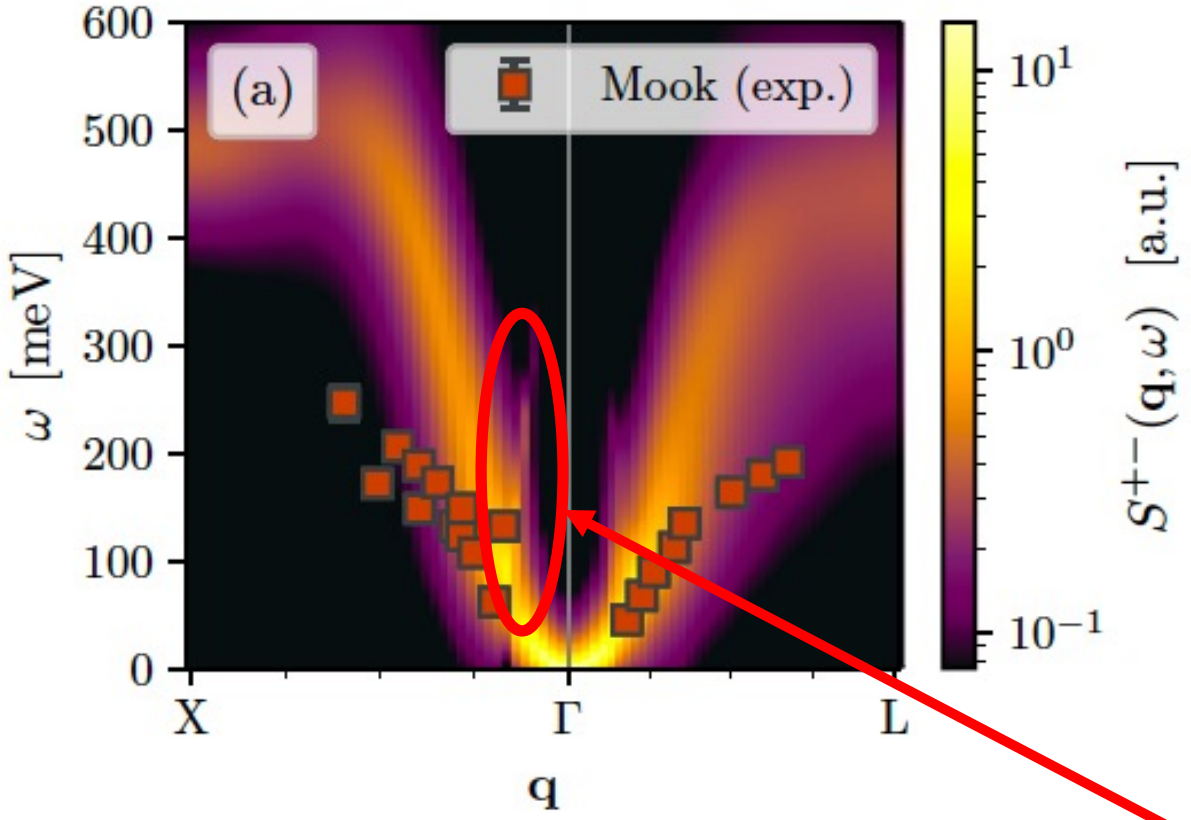

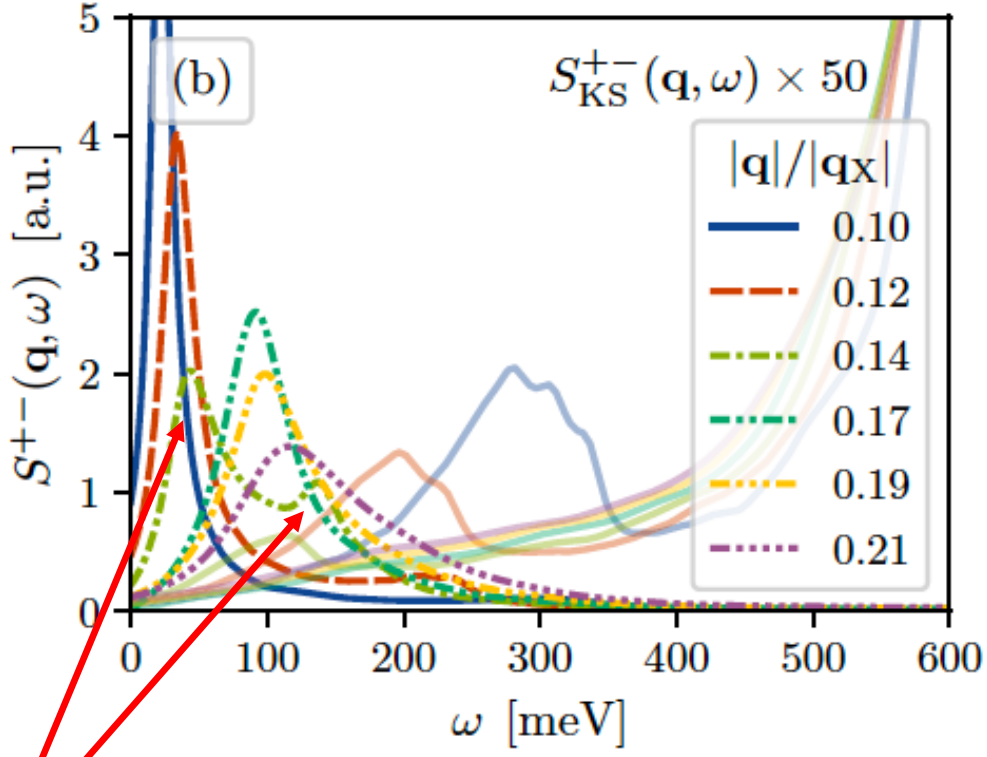

Coupling to Stoner continuum can yield non-Lorentzian spectral features

T. Skovhus and T. Olsen, *Phys. Rev. B* **103** 245110 (2021)

Conclusion

- Single-q magnetic order is easily pinned down by DFT
- Adding SOC (and assuming only bi-linear spin coupling) then rigorously determines the magnetic order
- Magnetic excitations may be determined from either
  - DFT and mapping to Heisenberg models
  - Time-dependent density functional theory (full spectral function)
  - Many-body perturbation theory (full spectral function)