NORDITA

Spin wave excitations of magnetic metalorganic materials

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Tartu, 17 September 2019

Collaborations

The Swedish QuEST for BIFROST and quantum materials

Experiment
Martin Månsson (KTH)
Yasmine Sassa (Chalmers)
Rasmus Toft Pedersen (DTU, ESS)

Theory
Alexander Balatsky (Nordita)
Johan Hellsvik (Nordita)
Olle Eriksson (Uppsala University)

Funding
The Swedish Research Council

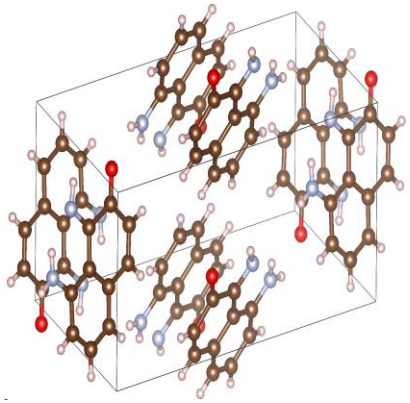
Vetenskapsrådet

The organic materials database (OMDB)

R. Matthias Geilhufe (Nordita)
Stanislav Borysov (Nordita, DTU)
Bart Olsthoorn (Nordita)
Roberto Díaz Pérez (Nordita)
Johan Hellsvik (Nordita)
David Carvalho (Nordita)
Alexander Balatsky (Nordita)

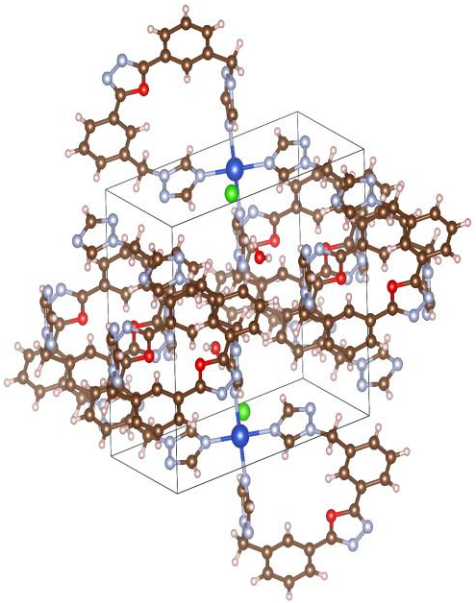
https://omdb.mathub.io

Why organics?



Properties

- strong correlations and electron interactions → complex phase diagrams
- softness → flexitronic
- infinite coordination space



Applications

- OLEDs, molecular qubits, spintronics, magnon spintronics, spin liquid physics, ...

The Organic Materials Database

Free to use:

https://omdb.mathub.io

Borysov, *et al., PLoS ONE,* 12(2), e0171501 (2017)

Electronic Structure

- Band structure, DOS

First dataset

- VASP, PBE
- ≈ 28, 000 materials

Second dataset

- VASP, SCAN+VdW
- (DFT-TS)
- in progress

Magnetic Structure

- Magnon spectra
- Magnetic ground state

First Dataset

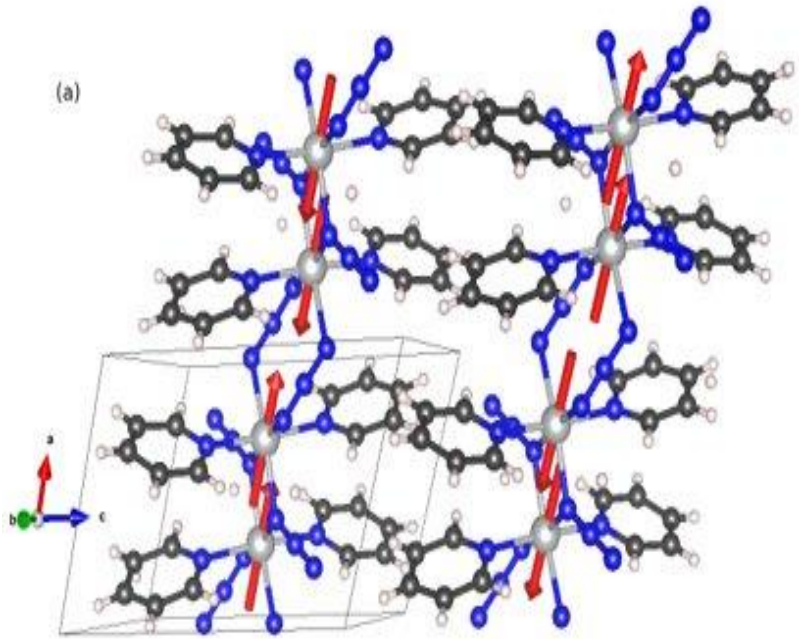
- RSPT
- linear spin-wave theory
- ≈ 100 materials

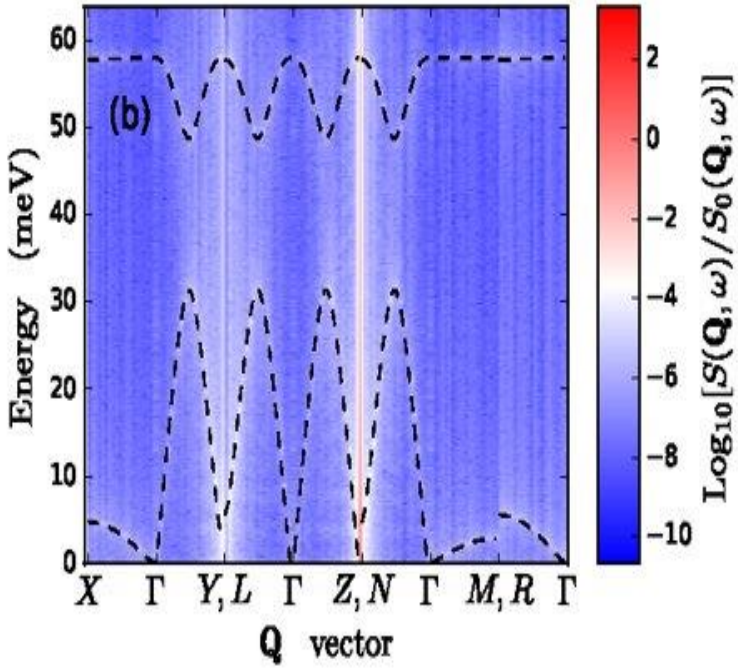
Hellsvik, *et al.,* arXiv 1907.01817

OMDB Community

1. provide/request services
2. upload your own results
3. ”Follow” materials

Magnetic Excitations of organic magnets





Organic magnetic material with exchange between magnetic metal ions (silver) mediated over organic ligands

Excitation spectra from multiscale ab initio modeling

Hellsvik, Díaz Pérez, Geilhufe, Månsson, and Balatsky, arXiv 1907.01817

Magnetic excitations on the OMDB

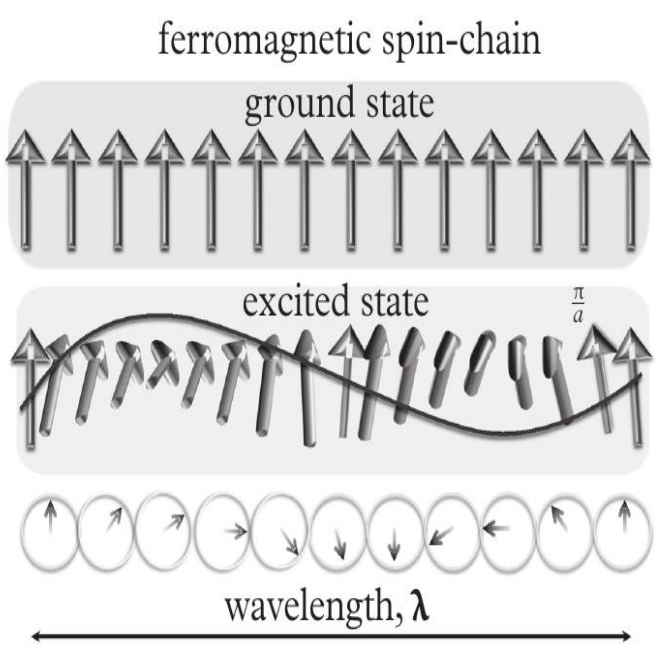
Scope: Materials informatics for magnetic excitations on the Organic Materials Database (OMDB)

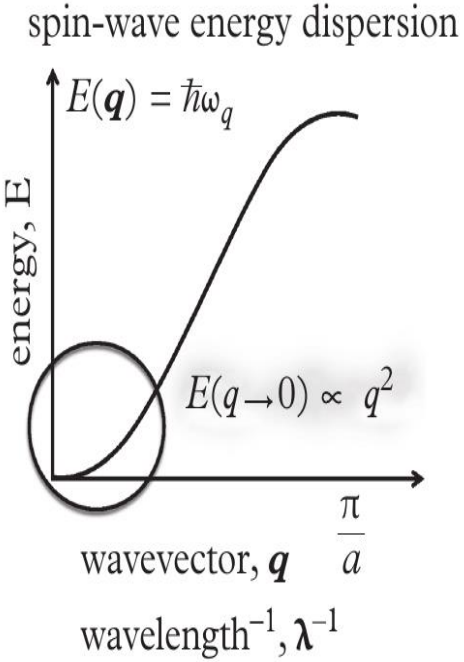
Physical entities: Magnetic ground states, interactions, and excitations spectra for crystalline solids

Ab initio dataset: High throughput calculations for spin Hamiltonians. Calculation of magnetic ground states and magnon spectra

Machine learning: Prediction of local magnetic properties: magnetic moments and Heisenberg interactions

Magnetic Hamiltonians and spin waves

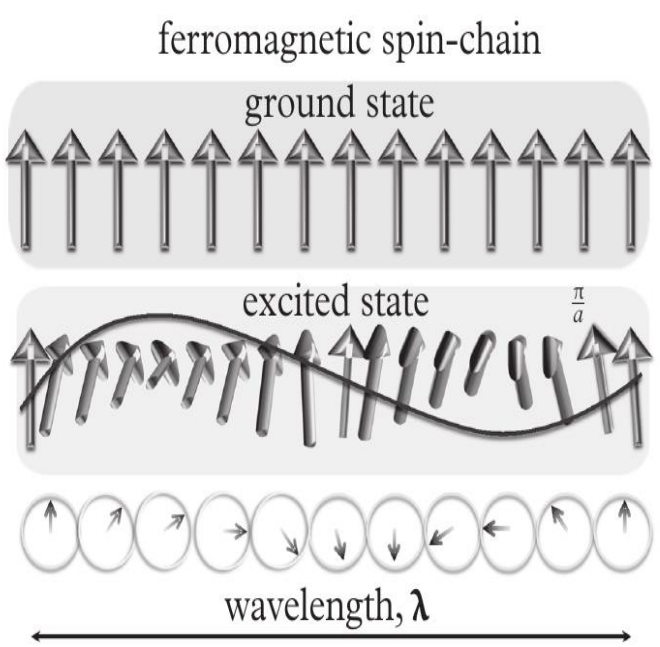


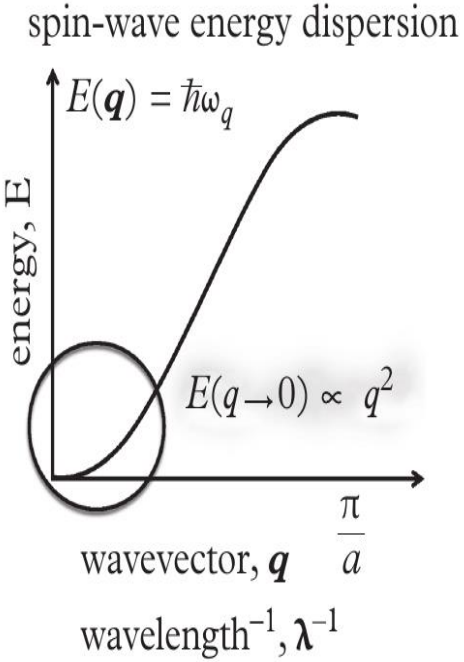


Magnetic Hamiltonians to model low energy magnetic excitations

$$\mathcal{H}_{\text{Heis}} = -\frac{1}{2}\sum_{i \neq j} \mathcal{J}_{ij}\mathbf{m}_i \cdot \mathbf{m}_j,$$

Magnetic Hamiltonians and spin waves





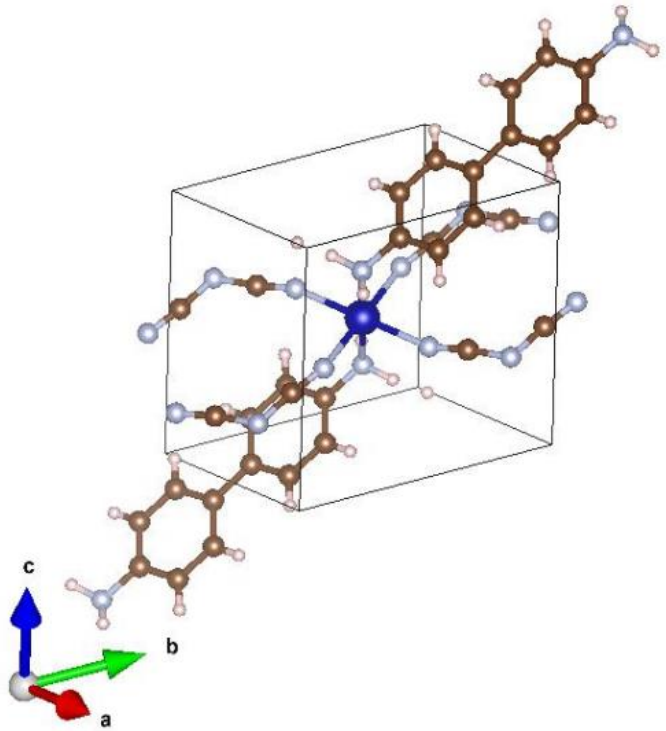
Magnetic Hamiltonians to model low energy magnetic excitations

$$\mathcal{H}_{\text{Heis}} = -\frac{1}{2}\sum_{i\neq j}\mathcal{J}_{ij}\mathbf{m}_i \cdot \mathbf{m}_j,$$

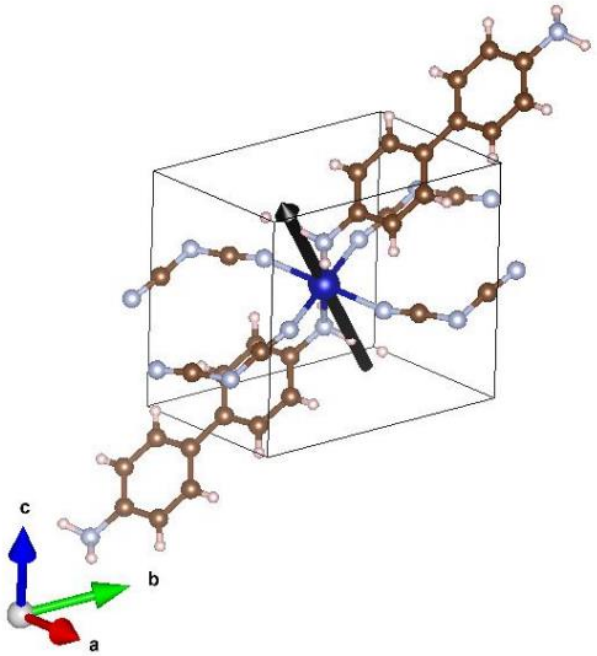
Dispersion relations ω(**q**) with linear spin wave theory

Dynamic structure factor S(**q**,ω) with atomistic spin dynamics (ASD) simulations

Magnetic moments $\mathbf{m}_i$ and Heisenberg interactions J_{ij}

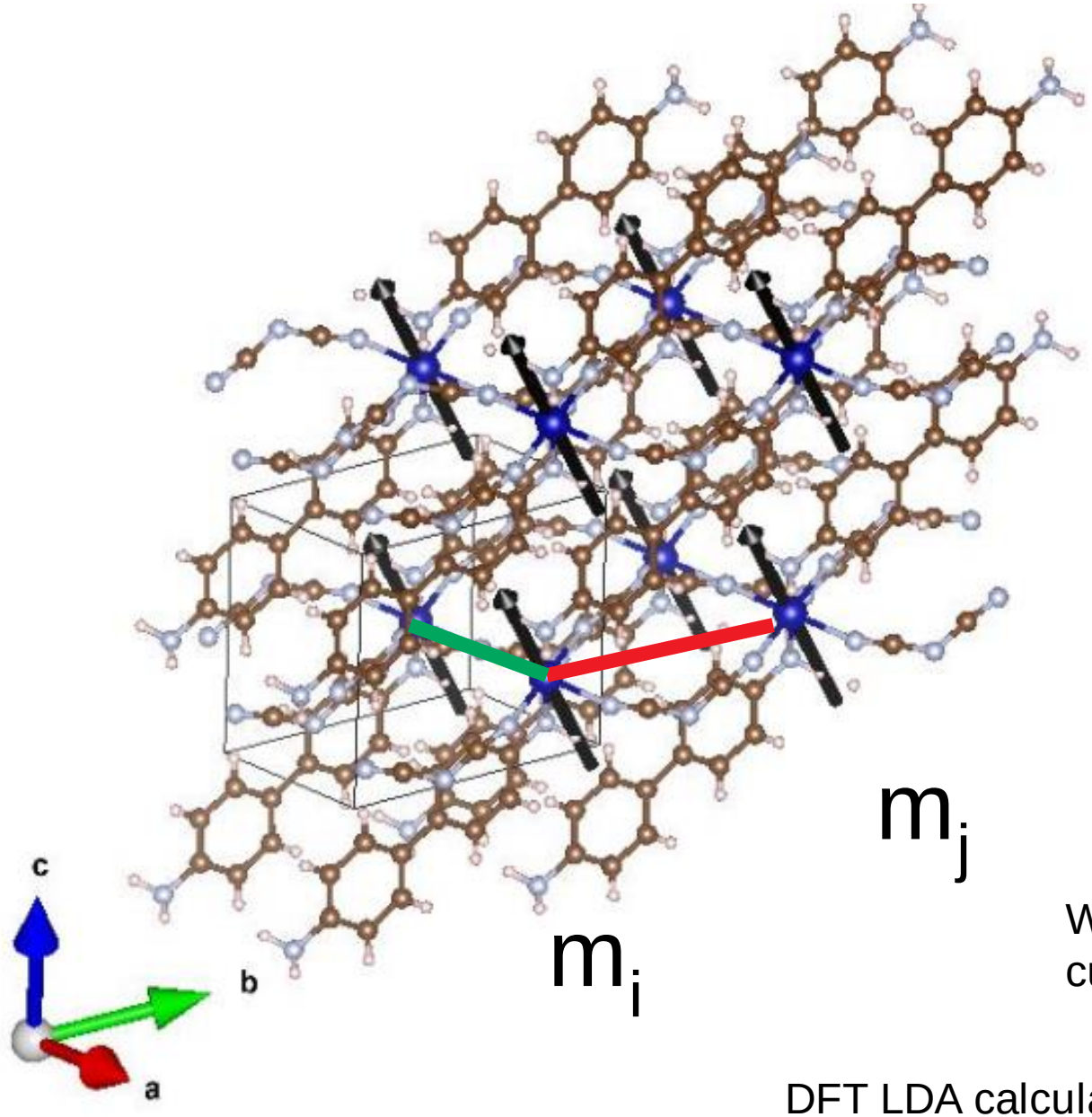


Chemical unit cell



magnetic sites m_i (>0.1 muB)

Magnetic moments $\mathbf{m}_i$ and Heisenberg interactions J_{ij}



$$\mathcal{H}_{\text{Heis}} = -\frac{1}{2}\sum_{i\neq j}\mathcal{J}_{ij}\mathbf{m}_i \cdot \mathbf{m}_j,$$

Nearest neighbour interaction J_{NN}

Next nearest neighbour interaction J_{NNN}

We consider interactions up to a cut-off radius r_c

DFT LDA calculations using the LKAG formula
Liechtenstein *et al.*, J. Mag. Mat **67**, 65 (1987)

The cyclopentadiene alkylation and nickel complex $C_{14}H_{23}Ni_{0.5}$

https://omdb.mathub.io/material/cod/4064866

Formula:
$C_{14}\ H_{23}\ Ni_{0.5}$
OMDB ID:
855
COD ID:
4064866

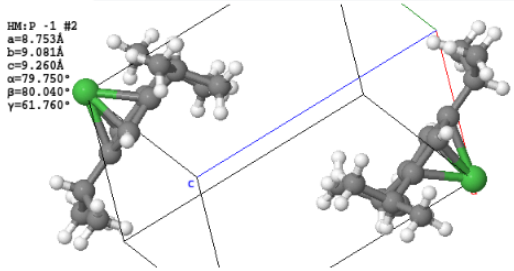
Publication details:
Cyclopentadiene Alkylation and Nickel Complexes with Tri-, Tetra-, or Pentaisopropylcyclopentadienide or an Even Bulkier Lithium Alkylcyclopentadienide

Publisher:
Organometallics, 2011, vol: 30, page: 6351

Version History:
No changes

Crystallographic Information

COD Data



Explore
load unitcell | load 8 unitcells

Interact
rotate to best view | default zoom
hide symmetry
spin on

a	8.7530(10)
b	9.0810(10)
c	9.2600(10)
α	79.750(10)
β	80.040(10)
γ	61.760(10)

Download cif file | COD link

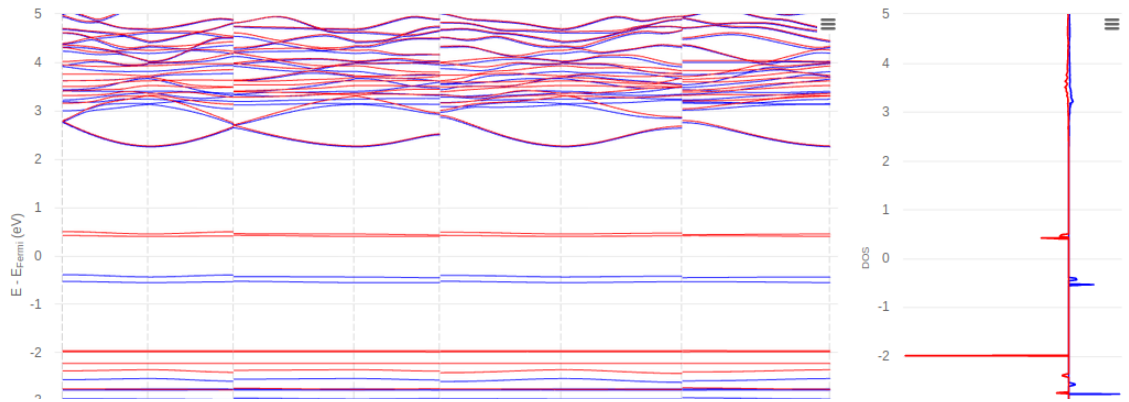
Symmetry properties

Hermann-Mauguin symmetry space group	P -1
Hall symmetry space group	-P 1
Space group IT number	2

Band structure and density of states

PBE

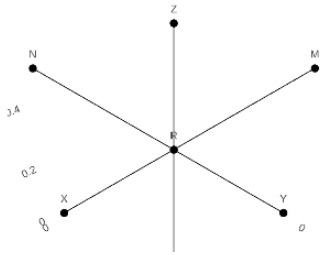
Select a range with the left mouse button to zoom in



Indirect band gap DFT GGA* (eV)	0.789
Magnetization density [μ_B/Å^3]	0.0031

* Warning! DFT is not very accurate in estimation of band gaps and tends to underestimate them.

Special points in the Brillouin zone



Formula:
C_{14} H_{23} $Ni_{0.5}$
OMDB ID:
855
COD ID:
4064866

Publication details:
Cyclopentadiene Alkylation and Nickel Complexes with Tri-, Tetra-, or Pentaisopropylcyclopentadienide or an Even Bulkier Lithium Alkylcyclopentadienide

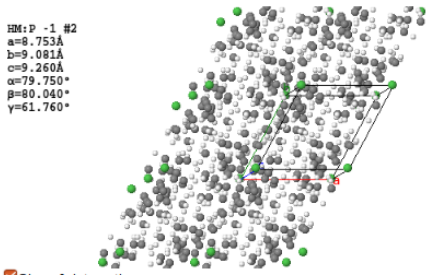
Publisher:
Organometallics, 2011, vol: 30, page: 6351

Version History:
No changes

J_{ij}
Ordered by magnitude

i	j	r [Å]	J_{ij} [meV]	Color
1	1	9.16	-0.06	■
1	1	8.75	-0.01	■
1	1	9.08	0.00	■
1	1	13.69	0.00	■

Visualize



Show J_{ij} interactions

Magnetic Moments

i	Species	Magnetic Moment [μ_B]
1	Ni	0.8350382

Input files for UppASD calculations

inpsd.dat | jfile_cart | momfile_cart | posfile_cart | qfile_cart

Community Contributions

Add your contribution

There isn't any community contribution for this material.

Services

Propose or request a new service

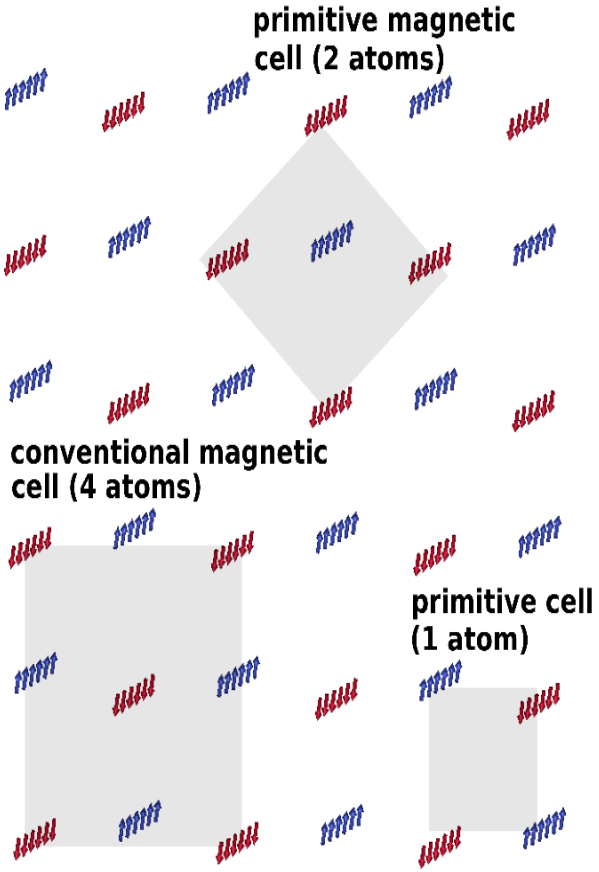
There isn't any service proposal or request for this material.

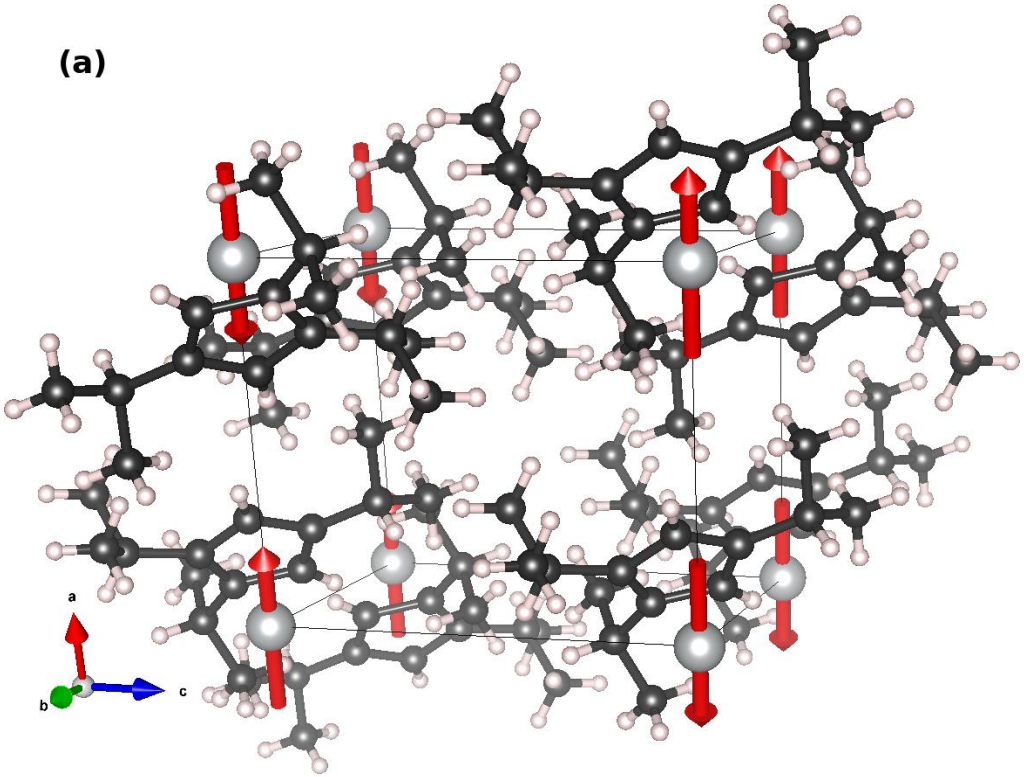
Similar Materials

Most similar materials with respect to DOS, using cosine distance:

ID (OMDB	ID (COD)	Formula	Space group H-M	Space group IT	Distance
24688	4323277	C_{26} H_{42} Ni O_4	P -1	2	72.87
16919	4324036	C_{12} H_{14} N_6 Ni	P -1	2	75.82
24386	4305333	C_{24} H_{36} N_{10} Ni	P -1	2	77.00
18946	8100332	C_8 H_{20} Ni O_8	P -1	2	80.77
27603	7052336	C_{30} H_{44} N_8 Ni	P -1	2	89.73
16917	4323279	C_{12} H_{18} Ni O_4	P -1	2	94.48
20173	2234546	C_{20} H_{16} N_{14} Ni	P -1	2	94.86

Ground state and primitive magnetic cell





Ground state obtained from atomistic spin dynamics quenching simulation down to T=0 K

Formula:
$C_{14}H_{23}Ni_{0.5}$

OMDB ID:
855

COD ID:
4064866

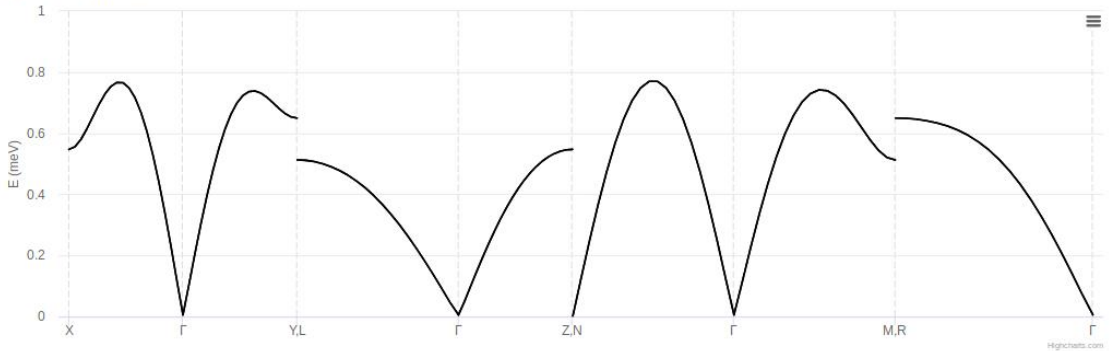
Publication details:
Cyclopentadiene Alkylation and Nickel Complexes with Tri-, Tetra-, or Pentaisopropylcyclopentadienide or an Even Bulkier Lithium Alkylcyclopentadienide

Publisher:
Organometallics, 2011, vol: 30, page: 6351

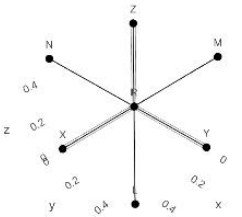
Version History:
No changes

Magnetic properties

Spin Wave Dispersion



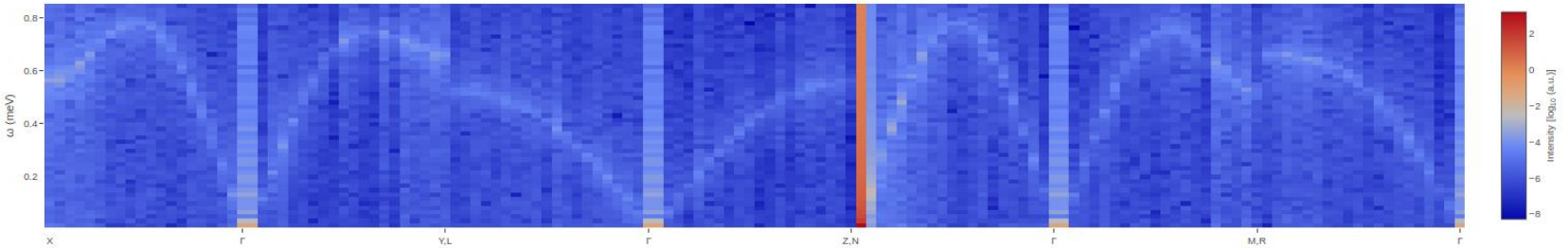
Special points in the Brillouin zone



LDA calculations with RSPt.

Absolute value of the dynamical structure factor S(q,ω)

For details see: arXiv 1907.01817

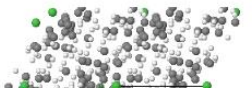


J_{ij}

Ordered by magnitude

i	j	r [Å]	J_{ij} [meV]	Color
1	1	9.16	-0.06	■

Visualize



Magnetic Moments

i	Species	Magnetic Moment [μ_B]
1	Ni	0.8350382

$C_6H_7Cl_3Ti$

Formula:
$C_6 H_7 Cl_3 Ti$
OMDB ID:
11695
COD ID:
2000232

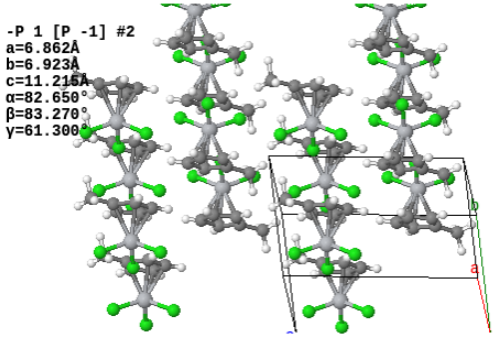
Publication details:
Structure of trichloro(\h^5^-methylcyclopentadienyl)titanium(IV)

Publisher:
Acta Crystallographica Section C, 1991, vol: 47, page: 2216

Version History:
No changes

Crystallographic Information

COD Data



Explore

load unitcell | load 8 unitcells

Interact

rotate to best view | default zoom

hide symmetry

spin on

a	6.8620(10)
b	6.923(2)
c	11.215(2)
α	82.650(10)
β	83.270(10)
γ	61.300(10)

Download cif file | COD link

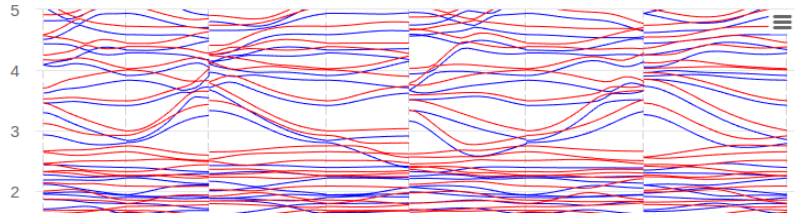
Symmetry properties

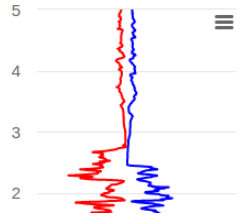
Hermann-Mauguin symmetry space group	P -1
Hall symmetry space group	-P 1
Space group IT number	

Band structure and density of states

PBE

Select a range with the left mouse button to zoom in





Indirect band gap DFT GGA* (eV)	0
Magnetization density [μ_B/Å^3]	0.0086

* Warning! DFT is not very accurate in estimation of band gaps and tends to underestimate them.

Special points in the Brillouin zone

Formula:
$C_6 H_7 Cl_3 Ti$

OMDB ID:
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COD ID:
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Publication details:
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Publisher:
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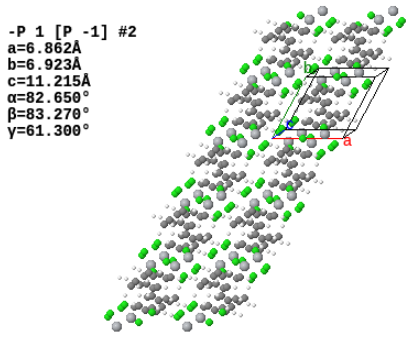
Version History:
No changes

J_{ij}
Ordered by magnitude

i	j	r [Å]	J_{ij} [meV]	Color
1	2	8.04	0.26	
2	2	6.92	0.08	
1	1	6.92	0.08	
1	2	7.92	-0.02	
2	2	7.03	-0.01	
1	1	7.03	-0.01	
1	2	5.57	0.01	
1	2	13.93	-0.01	
1	2	6.12	-0.01	
1	2	8.39	-0.01	

Visualize



Show J_{ij} interactions

Magnetic Moments

i	Species	Magnetic Moment [μ_B]
1	Ti	0.2242664
2	Ti	0.2242564

Input files for UppASD calculations

inpsd.dat | jfile_cart | momfile_cart | posfile_cart | qfile_cart

Community Contributions

Add your contribution

There isn't any community contribution for this material.

Services

Propose or request a new service

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Similar Materials

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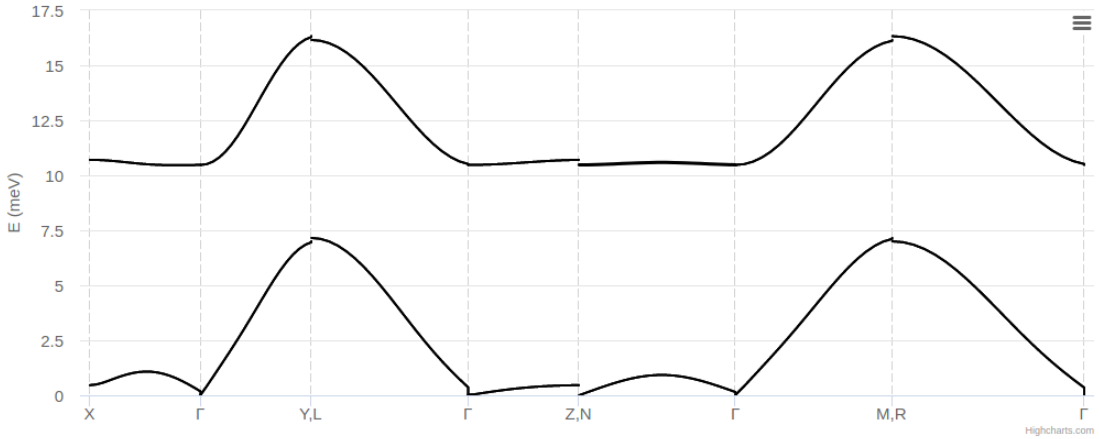
Publisher:
Acta Crystallographica Section C, 1991, vol: 47, page: 2216

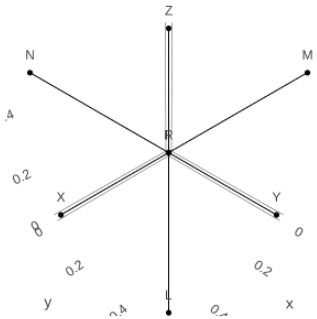
Version History:
No changes

Magnetic properties

Spin Wave Dispersion

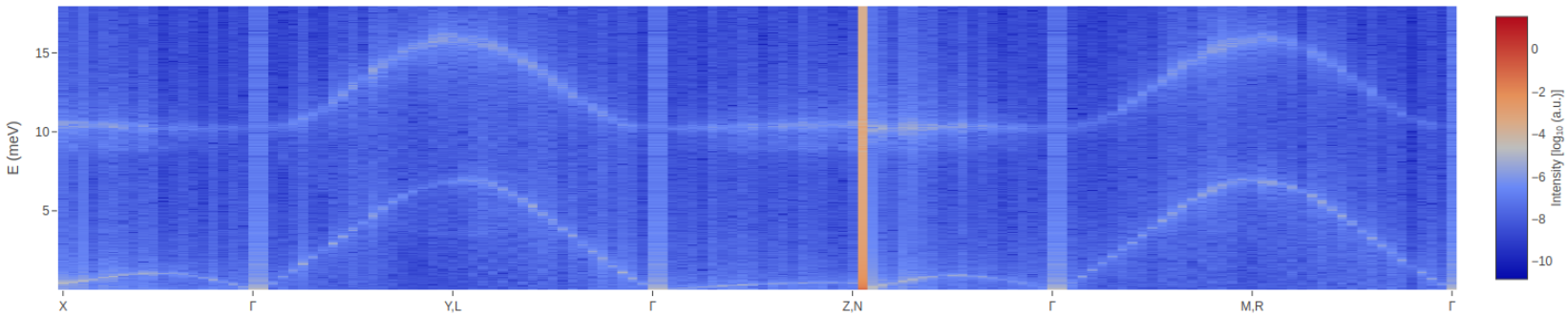


Special points in the Brillouin zone

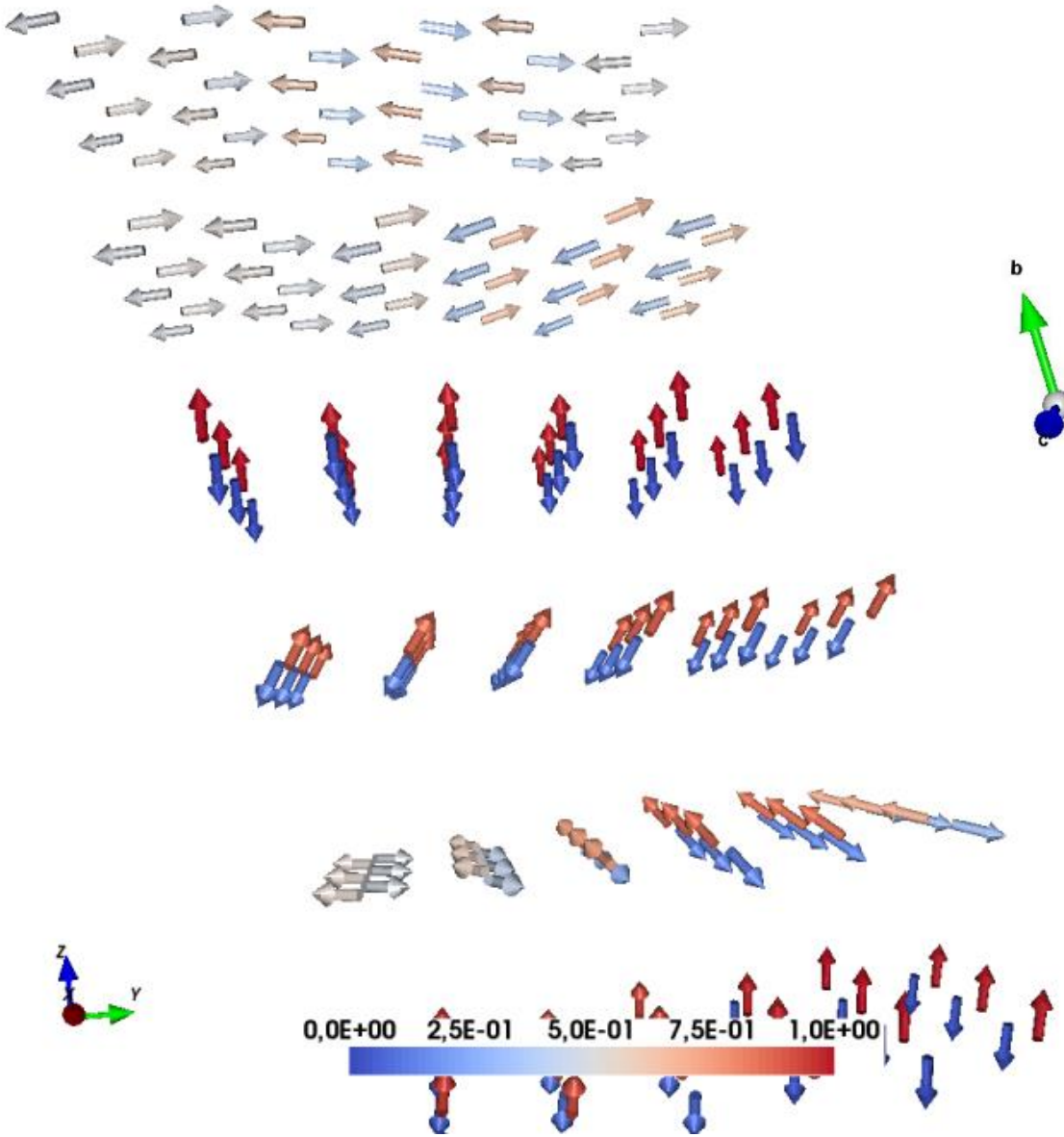


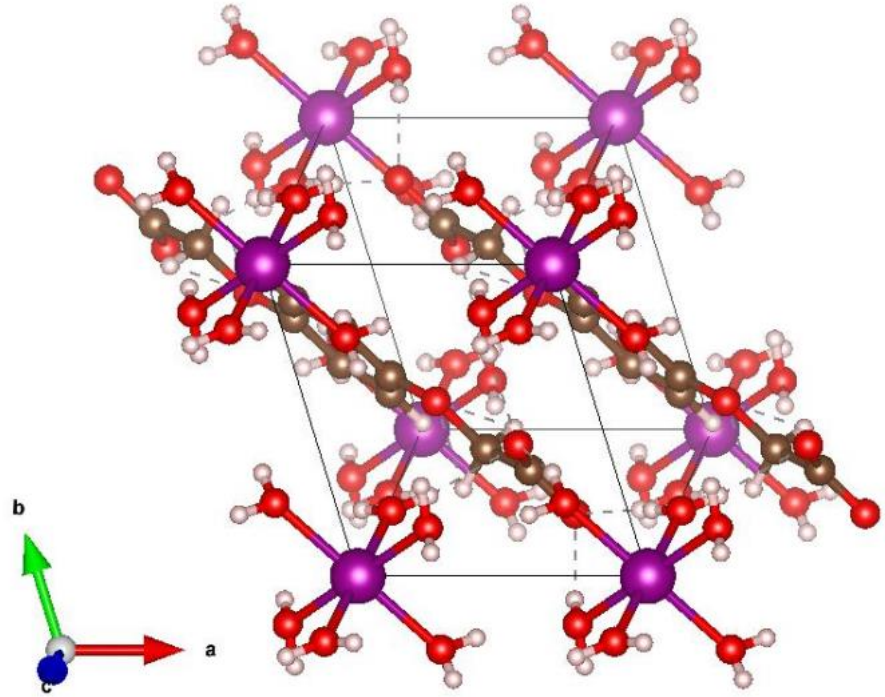
LDA calculations with RSPt.

Dynamical structure factor S(Q,ω)



Material COD 2203562

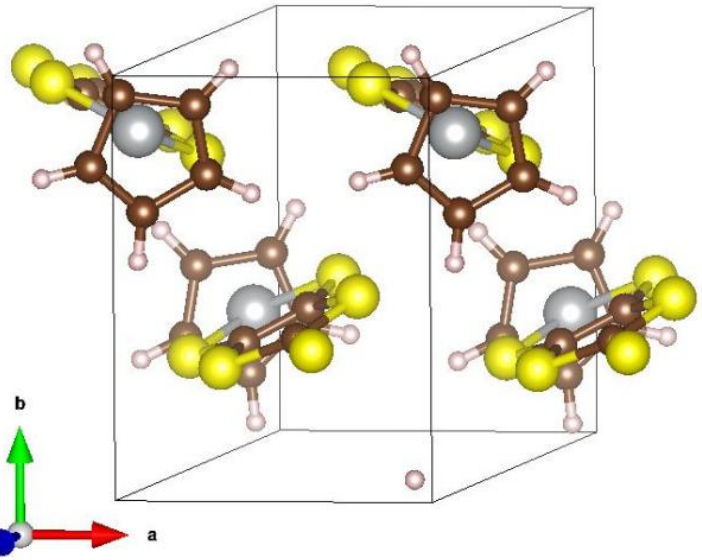


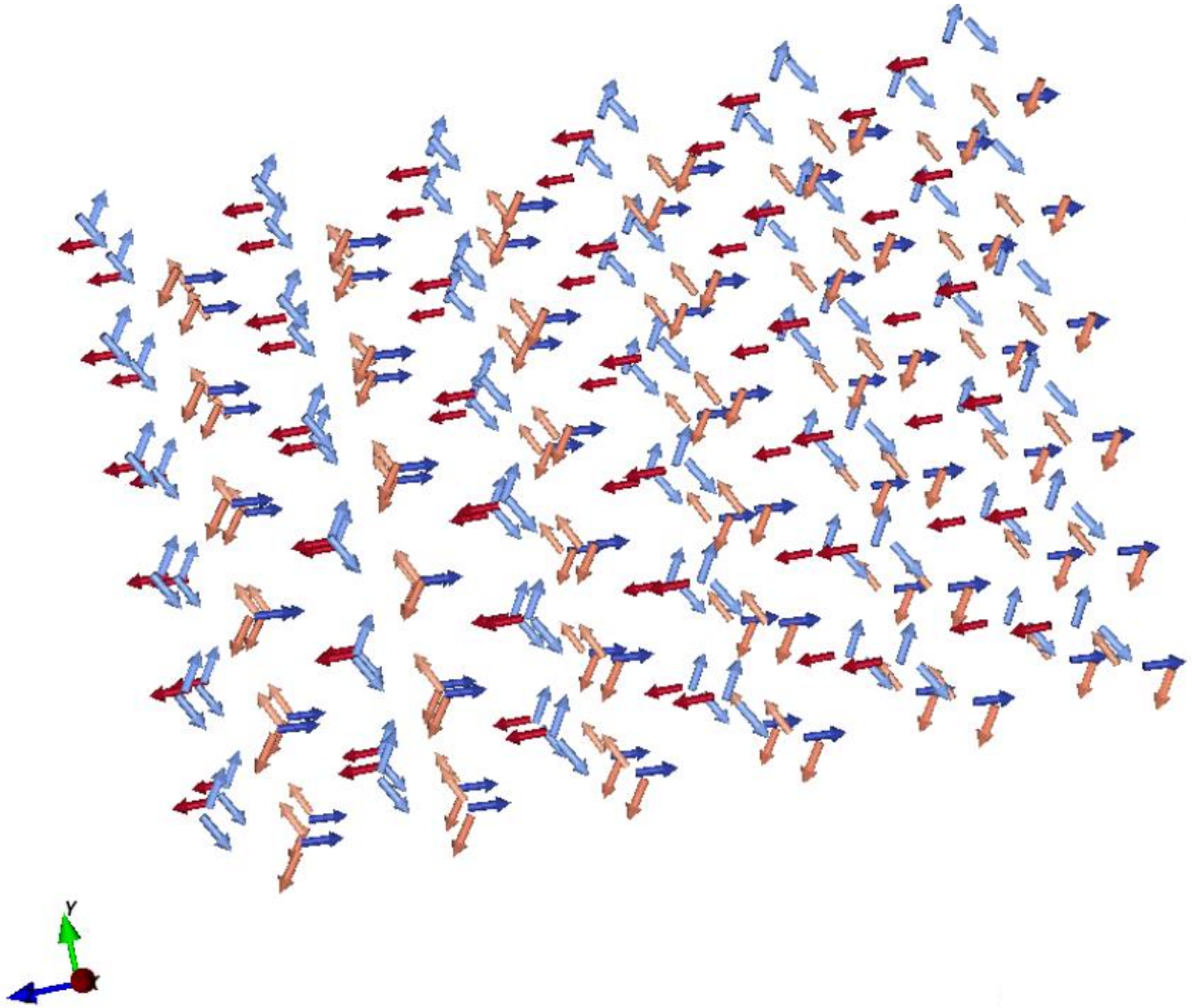


AFM spin spiral ordering

Modulated with incommensurate wave vector

Material COD 7008182

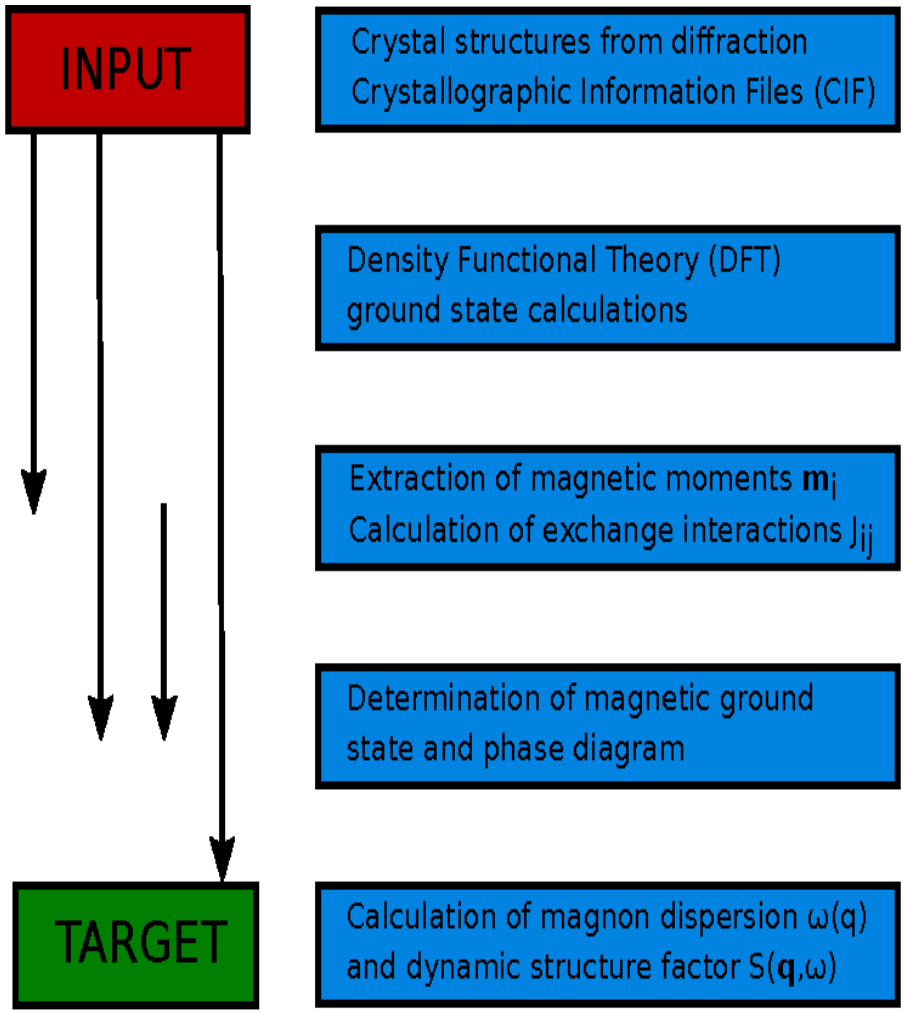




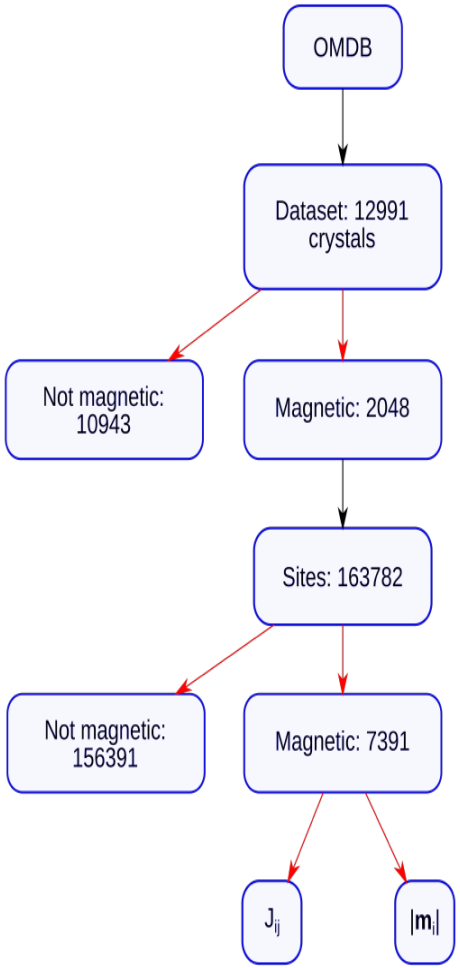
120 degree AFM configuration

Commensurate magnetic ordering?

Multiscale ab initio modeling & machine learning



Machine learning of magnetic properties



Challenge: Predict local properties of complex crystal structures

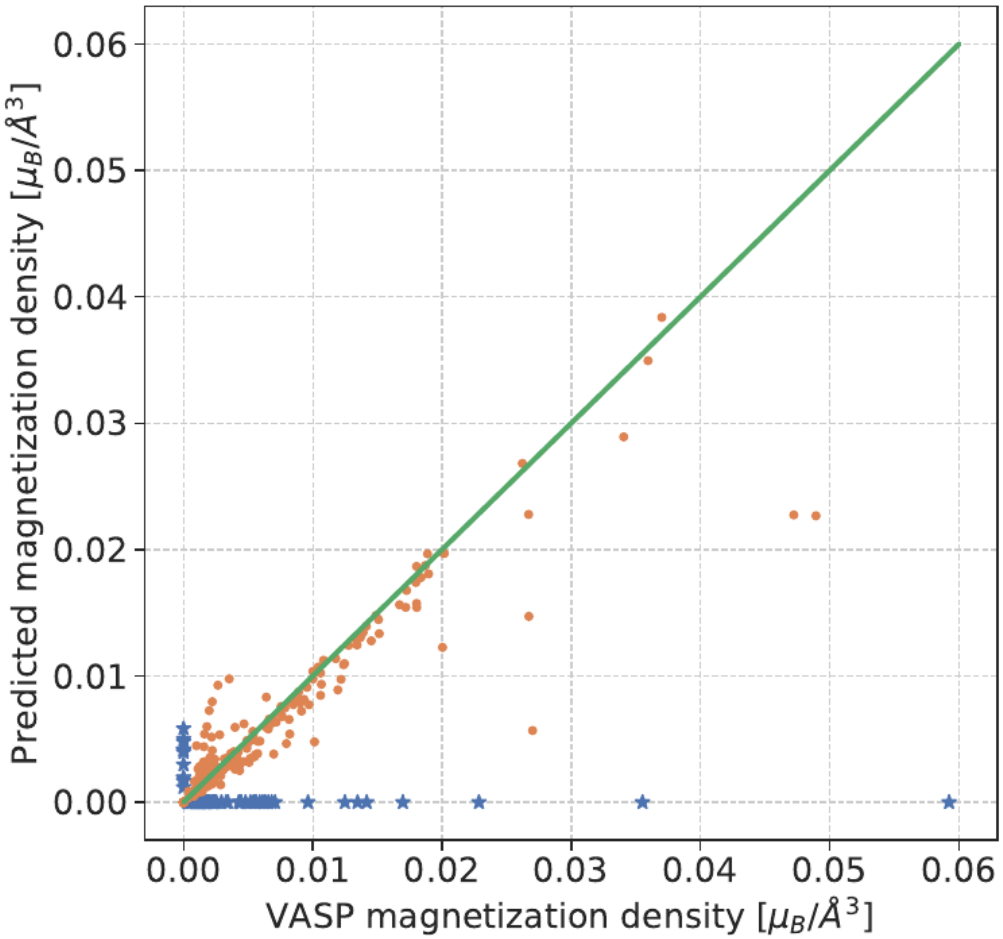
Target: Magnetic moments and Heisenberg interactions

Strategy:

1. Classification of crystals as magnetic or non-magnetic
2. Classification of atoms as magnetic or non-magnetic
3. Regression for $|\mathbf{m}_i|$ and J_{ij}

Roberto Díaz Pérez, MSc thesis, Stockholm University and Nordita (2019)
R. Díaz Pérez, R. M. Geilhufe, J. Hellsvik, and A. V. Balatsky, *in preparation* (2019).

Regression for magnetization density – machine learning



Performance for Radial Multi-Hot

Metric:

$$r^2 = 1 - \frac{\text{MSE}}{\text{VAR}}$$

where

MSE = Mean Square Error

VAR = Variance

For all data: r^2=0.67

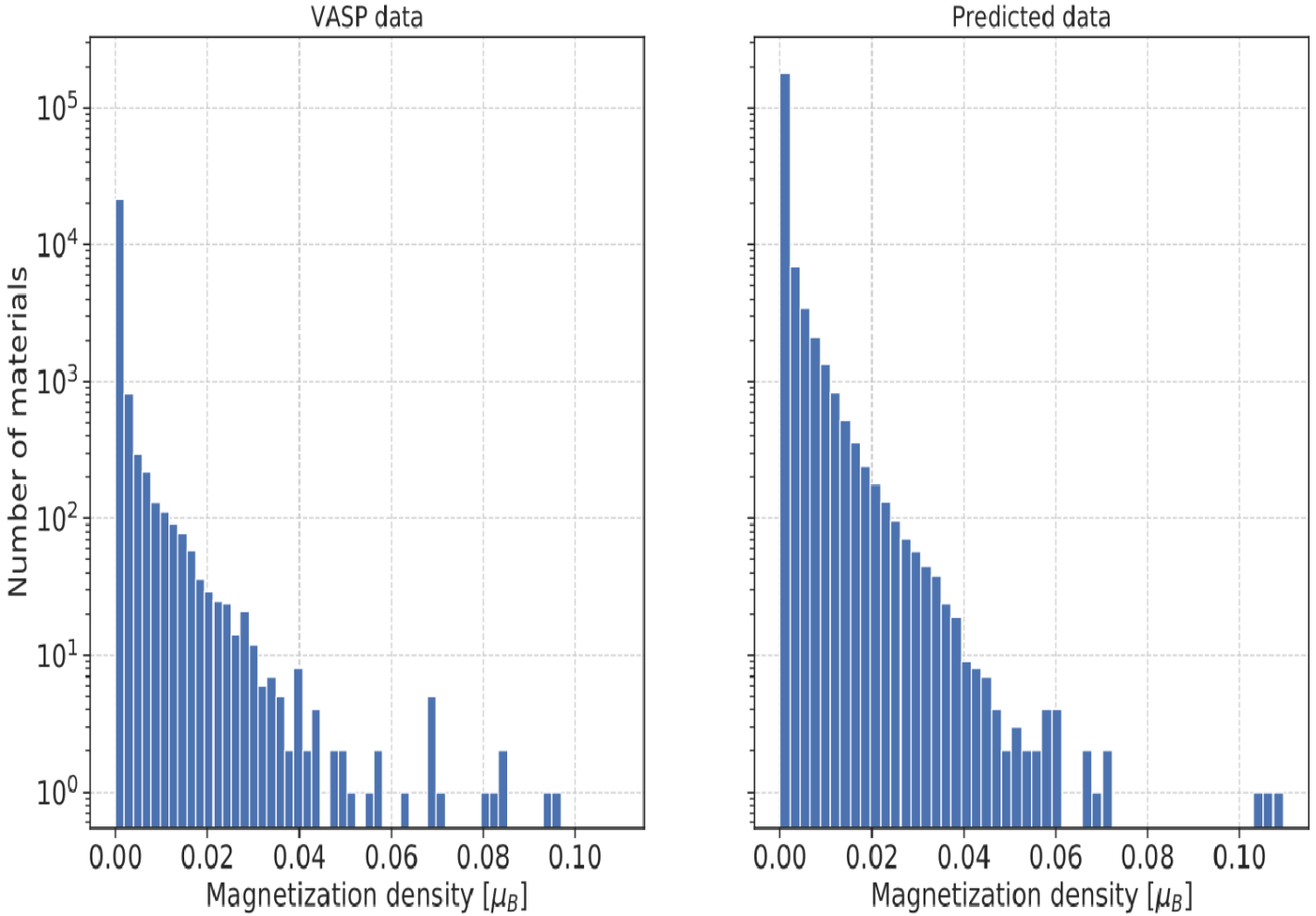
Blue asterisks represent missclassified materials

Removing missclassified data (magnetic or not magnetic)

r^2=0.89

which is a large improvement

Prediction of magnetization density



Distribution of DFT calculated magnetization density for 23,486 materials contained in the OMDB.

Distribution of machine learning predicted magnetization density for 196,471 materials.

Modeling of OMDB organic materials with spinW

Look for magnetic Hamiltonians posted on the OMDB

Set up the magnetic Hamiltonian in spinW

Calculate the spin wave spectra and dynamic structure factor with spinW

Compare with the spin wave and dynamic structure spectra available on the OMDB

Exercise: Calculate the spin wave spectra for the material https://omdb.mathub.io/material/cod/7018178

Formula:
$C_8 H_6 Co N_4 S_2$

OMDB ID:
34552

COD ID:
7018178

Publication details:
Weak ferromagnetism in chiral diamond-like neutral networks: Mn(2-pymS)(2) and Co(2-pymS)(2) (2-pymSH = 2-mercaptopyrimidine).

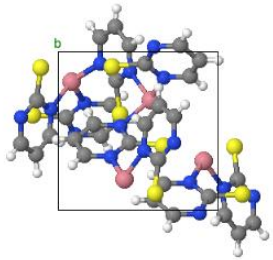
Publisher:
Dalton transactions (Cambridge, England : 2003), 2012, vol: 41, page: 2626

Version History:
No changes

Crystallographic Information

COD Data

```
HM:P 21 21 21 #19
a=7.792Å
b=7.792Å
c=16.509Å
α=90.000°
β=90.000°
γ=90.000°
```



Explore

load unitcell | load 8 unitcells

Interact

rotate to best view | default zoom

☐ hide symmetry

☐ spin on

a	7.7915(3)
b	7.7915(3)
c	16.5088(9)
α	90.00
β	90.00
γ	90.00

Download cif file | COD link

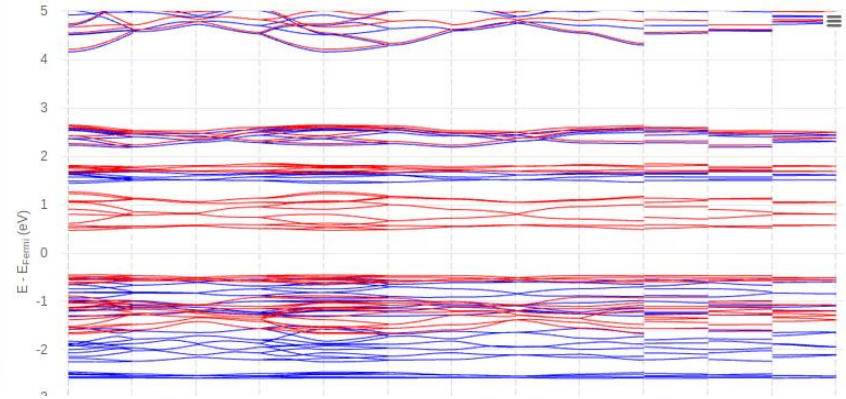
Symmetry properties

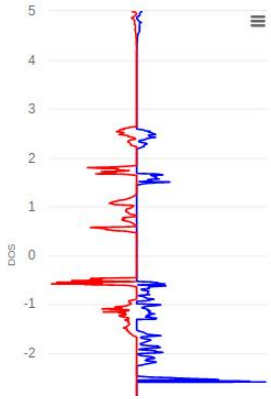
Hermann-Mauguin symmetry space group	P 21 21 21
Hall symmetry space group	P 2ac 2ab
Space group IT number	19

Band structure and density of states

PBE

Select a range with the left mouse button to zoom in

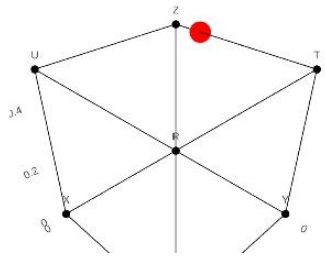




Indirect band gap DFT GGA* (eV)	0.9234
Magnetization density [μ_B/Å^3]	0.012

* Warning! DFT is not very accurate in estimation of band gaps and tends to underestimate them.

Special points in the Brillouin zone



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Version History:
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α=90.000°
β=90.000°
γ=90.000°
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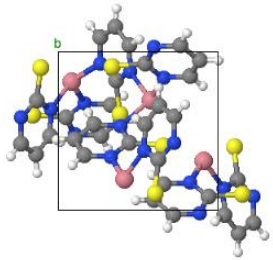

Explore
load unitcell | load 8 unitcells

Interact
rotate to best view | default zoom
hide symmetry
spin on

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α	90.00
β	90.00
γ	90.00

Download cif file | COD link

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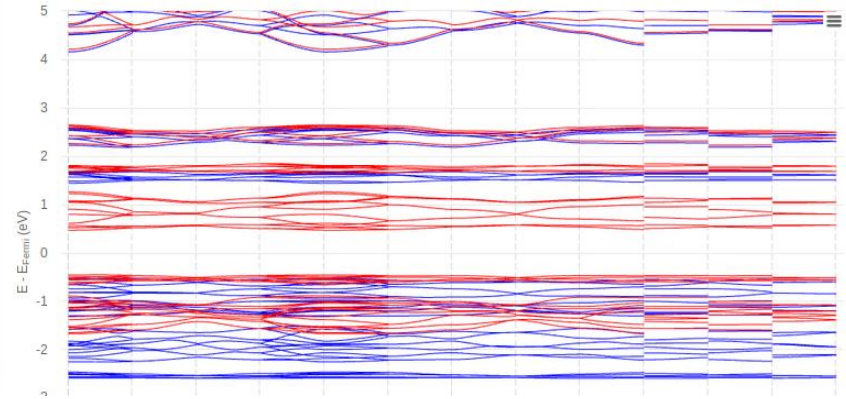
Hall symmetry space group	P 2ac 2ab
Space group IT number	19

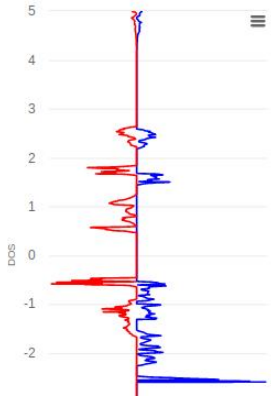
Input for spinW

Band structure and density of states

PBE

Select a range with the left mouse button to zoom in





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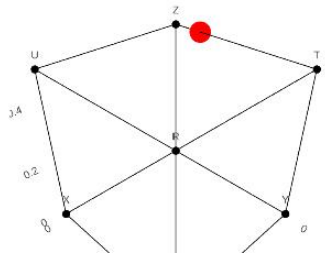
Magnetization density [μ_B/Å^3]	0.012

* Warning! DFT is not very accurate in estimation of band gaps and tends to underestimate them.

Special points in the Brillouin zone



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$C_8 H_6 Co N_4 S_2$
OMDB ID:
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COD ID:
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Publication details:
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Publisher:
Dalton transactions (Cambridge, England : 2003), 2012, vol: 41, page: 2626

Version History:
No changes

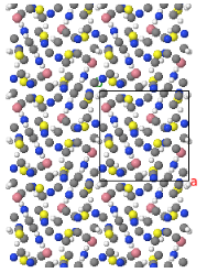
J_{ij}

Ordered by magnitude

i	j	r [Å]	J_{ij} [meV]	Color
1	4	5.80	-6.92	
3	2	5.80	-6.92	
1	3	5.77	-6.90	
2	4	5.77	-6.90	
1	2	10.18	0.08	
4	3	10.18	0.08	
2	1	9.15	0.07	
3	4	9.15	0.07	
1	2	9.91	0.05	
3	4	9.91	0.05	

Visualize

HM:P 21 21 21 #19
a=7.792Å
b=7.792Å
c=16.509Å
α=90.000°
β=90.000°
γ=90.000°



Show J_{ij} interactions

Magnetic Moments

i	Species	Magnetic Moment [μ_B]
1	Co	1.6307791
2	Co	1.630778
3	Co	1.6307789
4	Co	1.6307775

Input files for UppASD calculations

inpsd.dat | jfile_cart | momfile_cart | posfile_cart | qfile_cart

Community Contributions

Add your contribution

There isn't any community contribution for this material.

Services

Propose or request a new service

There isn't any service proposal or request for this material.

Similar Materials

Most similar materials with respect to DOS, using cosine distance:

ID (OMDB	ID (COD)	Formula	Space group H-M	Space group IT	Distance
137080	4075767	$C_5 H_5 Co N_2 S_2$	P 1 21/c 1	14	150.90
35994	7027336	$C_3 H_{14} Co N_2 O_8 P_2$	P 21 21 21	19	200.48
35963	2013643	$C_6 H_{12} Cl_2 Co N_4 O_2$	P b c a	61	217.11
139372	4077422	$C_{13} H_{18} Cl Ni P$	P 21 21 21	19	315.09

Formula:
$C_8 H_6 Co N_4 S_2$
OMDB ID:
34552
COD ID:
7018178

Publication details:
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Version History:
No changes

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Ordered by magnitude

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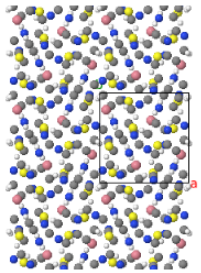
3	2	5.80	-6.92	
1	3	5.77	-6.90	
2	4	5.77	-6.90	
1	2	10.18	0.08	
4	3	10.18	0.08	
2	1	9.15	0.07	
3	4	9.15	0.07	
1	2	9.91	0.05	
3	4	9.91	0.05	

Visualize

HM:P 21 21 21 #19
a=7.792Å
b=7.792Å
c=16.509Å
α=90.000°
β=90.000°
γ=90.000°



Show J_{ij} interactions

Magnetic Moments

i	Species	Magnetic Moment [μ_B]
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2	Co	1.630778
3	Co	1.6307789
4	Co	1.6307775

Input files for UppASD calculations

inpsd.dat | jfile_cart | momfile_cart | posfile_cart | qfile_cart

Input for spinW

Community Contributions

Add your contribution

There isn't any community contribution for this material.

Services

Propose or request a new service

There isn't any service proposal or request for this material.

Similar Materials

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ID (OMDB	ID (COD)	Formula	Space group H-M	Space group IT	Distance
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35994	7027336	$C_3 H_{14} Co N_2 O_8 P_2$	P 21 21 21	19	200.48
35963	2013643	$C_6 H_{12} Cl_2 Co N_4 O_2$	P b c a	61	217.11
139372	4077422	$C_{13} H_{18} Cl Ni P$	P 21 21 21	19	315.09

Compare your spectra with graphs on https://omdb.mathub.io/material/cod/7018178

Formula:
$C_8 H_6 Co N_4 S_2$

OMDB ID:
34552

COD ID:
7018178

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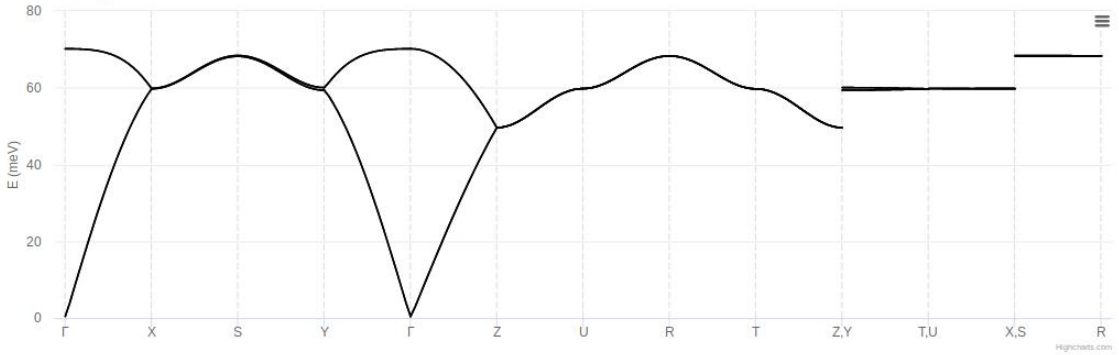
Publisher:
Dalton transactions (Cambridge, England : 2003), 2012, vol: 41, page: 2626

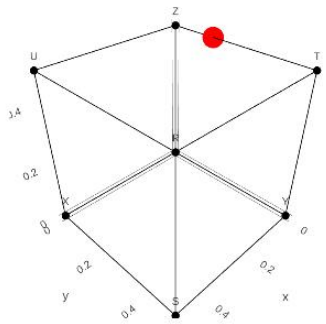
Version History:
No changes

Magnetic properties

Spin Wave Dispersion



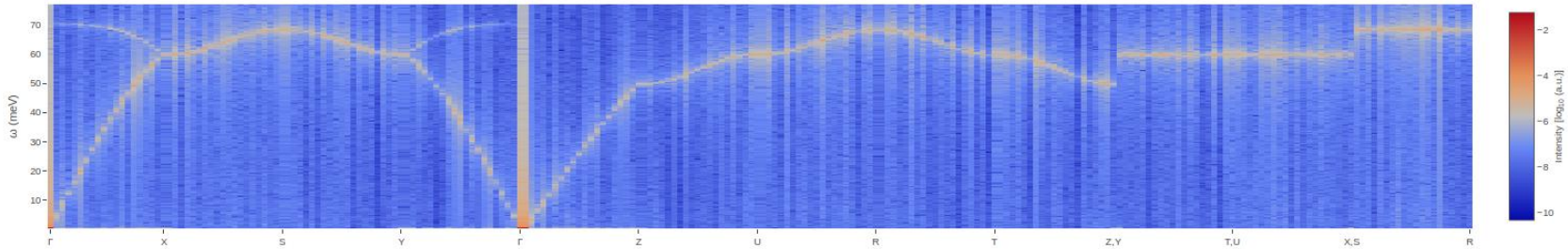
Special points in the Brillouin zone



LDA calculations with RSPt.

Absolute value of the dynamical structure factor S(q,ω)

For details see: arXiv 1907.01817

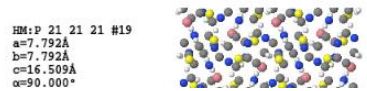


J_{ij}

Ordered by magnitude

i	j	r [Å]	J_{ij} [meV]	Color
1	4	5.80	-6.92	■

Visualize



Magnetic Moments

i	Species	Magnetic Moment [μ_B]
1	Co	1.6307791
2	Co	1.630778

Exercise: Calculate spin wave spectra for the material https://omdb.mathub.io/material/cod/7203358

OMDB Home Browse Search Machine Learning Team Account (2) About

Formula:
$C_4 H_6 Mn O_6$
OMDB ID:
22305
COD ID:
7203358

Publication details:
An approach to chiral magnets using ?-hydroxycarboxylates

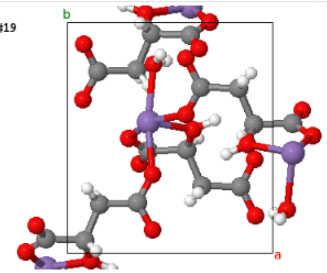
Publisher:
Journal of Materials Chemistry, 2006, vol: 16, page: 2715

Version History:
No changes

Crystallographic Information

COD Data

HM:P 21 21 21 #19
a=7.988Å
b=8.998Å
c=9.029Å
α=90.000°
β=90.000°
γ=90.000°



Explore
load unitcell | load 8 unitcells

Interact
rotate to best view | default zoom
hide symmetry
spin on

a	7.9880(10)
b	8.9980(10)
c	9.0290(10)
α	90.00
β	90.00
γ	90.00

Download cif file | COD link

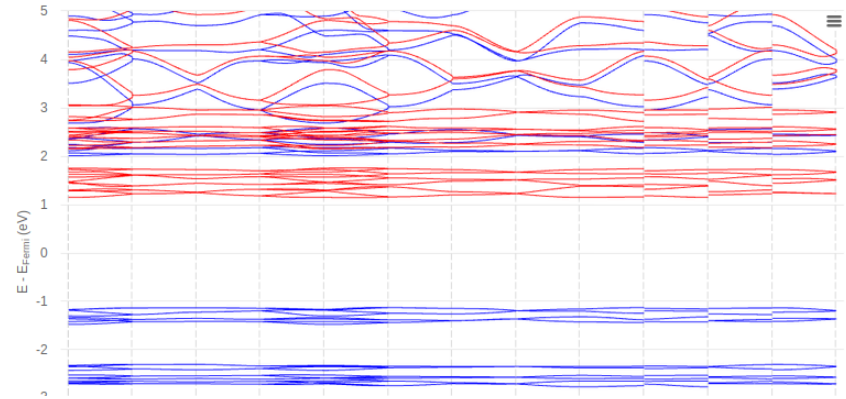
Symmetry properties

Hermann-Mauguin symmetry space group	P 21 21 21
Hall symmetry space group	P 2ac 2ab
Space group IT number	19

Band structure and density of states

PBE

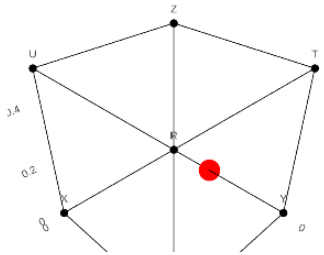
Select a range with the left mouse button to zoom in



Indirect band gap DFT GGA* (eV)	2.2726
Magnetization density [μ_B/Å^3]	0.0308

* Warning! DFT is not very accurate in estimation of band gaps and tends to underestimate them.

Special points in the Brillouin zone



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COD ID:
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An approach to chiral magnets using ?-hydroxycarboxylates

Publisher:
Journal of Materials Chemistry, 2006, vol: 16, page: 2715

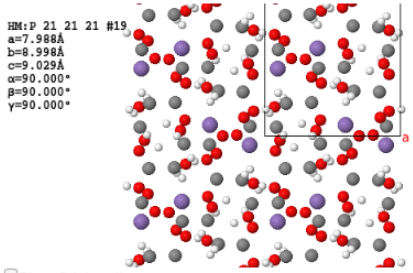
Version History:
No changes

J_{ij}

Ordered by magnitude

i	j	r [Å]	J_{ij} [meV]	Color
2	3	5.40	-0.37	
4	1	5.40	-0.37	
2	1	5.24	-0.30	
3	4	5.24	-0.30	
1	3	5.55	-0.03	
4	2	5.55	-0.03	
2	1	7.32	-0.01	
4	3	7.32	-0.01	
3	2	8.10	-0.01	
4	1	8.10	-0.01	

Visualize



Show J_{ij} interactions

Magnetic Moments

i	Species	Magnetic Moment [μ_B]
1	Mn	2.2329593
2	Mn	2.2329596
3	Mn	2.2329596
4	Mn	2.2329595

Input files for UppASD calculations

inpsd.dat | jfile_cart | momfile_cart | posfile_cart | qfile_cart

Community Contributions

Add your contribution

There isn't any community contribution for this material.

Services

Propose or request a new service

There isn't any service proposal or request for this material.

Similar Materials

Most similar materials with respect to DOS, using cosine distance:

ID (OMDB	ID (COD)	Formula	Space group H-M	Space group IT	Distance
22305	7203358	C_4 H_6 Mn O_6	P 21 21 21	19	0.00
27442	4331682	C_6 H_{10} Pd S_4	P 4/n :2	85	0.00
34622	4511809	C_6 H_{10} Co N_2 O_6	P 21 21 21	19	0.01
21298	7102783	C_2 H_6 O_6 Zn	P 1 21/c 1	14	0.01

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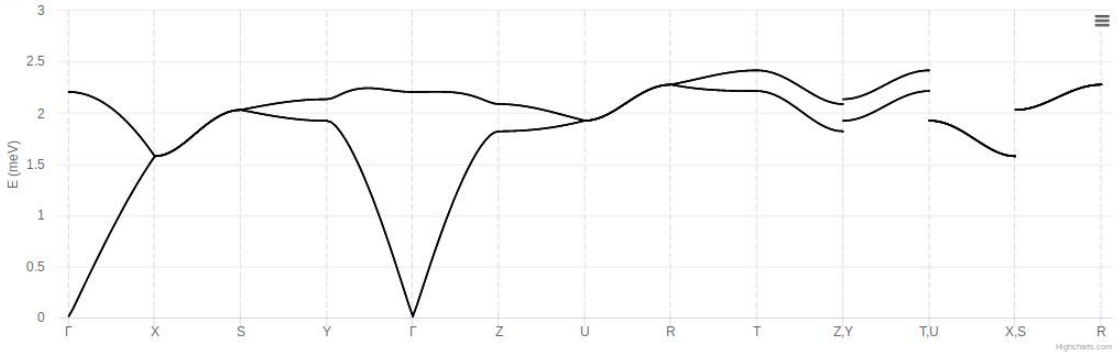

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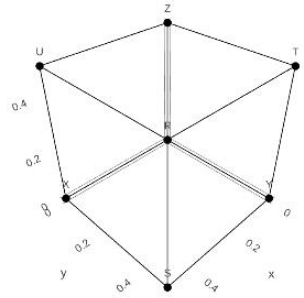
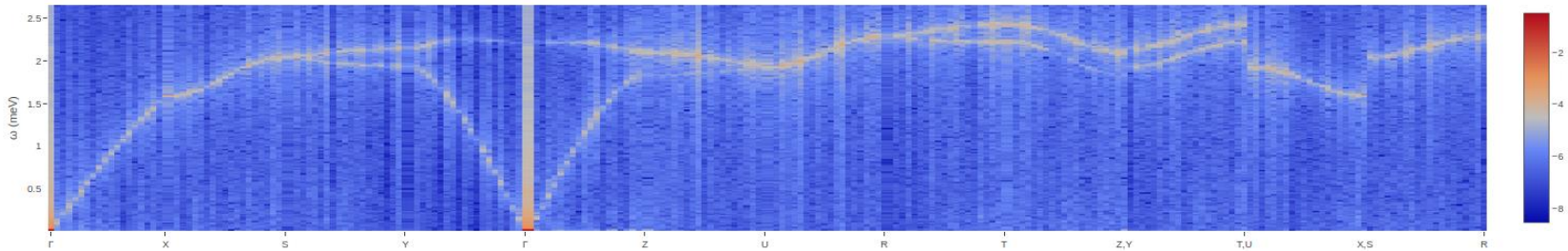


LDA calculations with RSPt.

Absolute value of the dynamical structure factor S(q,ω)

For details see: arXiv 1907.01817



J_{ij}

Ordered by magnitude

i	j	r [Å]	J_{ij} [meV]	Color
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Visualize

Magnetic Moments

i	Species	Magnetic Moment [μ_B]
1	Mn	2.2329593
2	Mn	2.2329596

Conclusions

Extending the OMDB to magnetic excitations

High throughput calculation of magnetic Hamiltonians and spin wave spectra

Machine learning for site-specific magnetic properties

Exercises on spin wave spectra for organic materials using spinW