AMCHECK: A TOOL TO CHECK WHETHER A COMPENSATED COLLINEAR MAGNETIC MATERIAL IS ANTIFERRO- OR ALTERMAGNETIC

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Introduction

Up to now only a limited amount of altermagnetic materials were reported and a tool to predict if a given material is an altermagnet or not would be of great use for seeking new altermagnetic candidates. Utilizing the fact that the magnetic moment compensation in these systems is driven by symmetry, we developed a program/library that allows to check if the given material is an altermagnet by using the information about its crystal structure and magnetic pattern.

Assumptions

- Magnetic compensation happens within each crystallographic orbit, i.e. ferrimagnets are excluded.
- Only collinear magnets are of interest.
- Space and spin coordinates are decoupled.
- Spin is a pseudoscalar quantity, i.e merely "up" or "down" and not a pseudovector.

Antiferromagnet vs Altermagnet

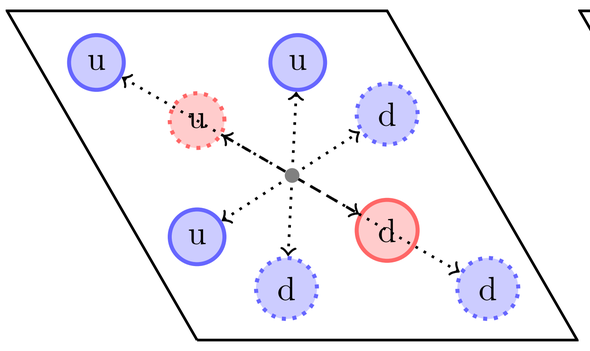

Fig. 1: Antiferromagnetic spin pattern.

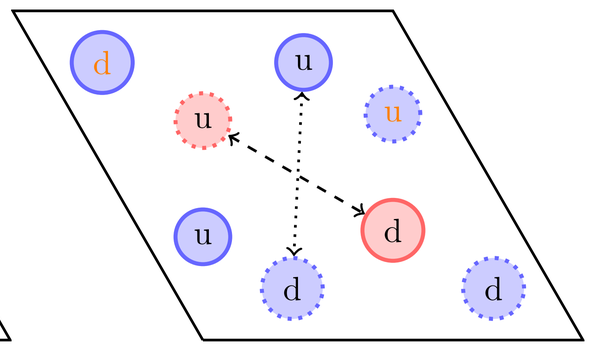

Fig. 2: Altermagnetic spin pattern.

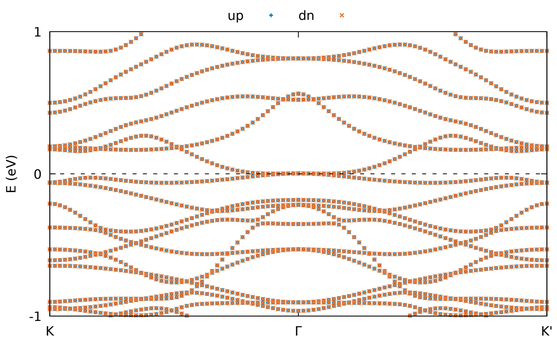

Fig. 3: Bands are degenerate.

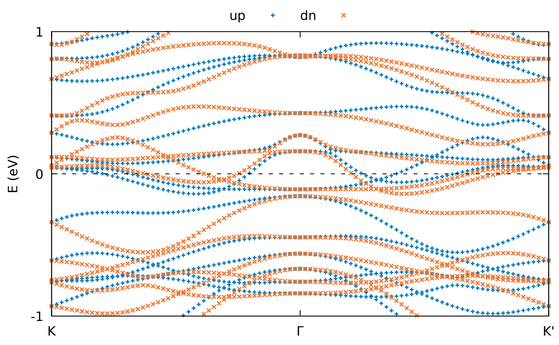

Fig. 4: Band splitting is present.

Using as a library

```
from amcheck import is_altermagnet

symmetry_operators = [(np.array([[-1,  0,  0],
                                 [ 0, -1,  0],
                                 [ 0,  0, -1]],
                                dtype=int),
                       np.array([0.0, 0.0, 0.0])),
                       # for compactness reasons,
                       # other symmetry operations are
                       # omitted from this example
                       ]
positions = np.array([[0.156793, 0.313586, 0.75],
                      [0.843207, 0.686414, 0.25],
                      [0.686414, 0.843207, 0.75],
                      [0.313586, 0.156793, 0.25],
                      [0.156793, 0.843207, 0.75],
                      [0.843207, 0.156793, 0.25],
                      [0.333333, 0.666667, 0.25],
                      [0.666667, 0.333333, 0.75]])
equiv_atoms = np.array([0, 0, 0, 0, 0, 0, 6, 6])
chem_symbols = ['Mn', 'Mn', 'Mn', 'Mn', 'Mn', 'Mn',
                'Fe', 'Fe']
spins = ['u', 'u', 'u', 'd', 'd', 'd', 'u', 'd']
is_altermagnet(symmetry_operators, positions, equiv_atoms,
               chem_symbols, spins)
```

Idea

Action of spin flip operator: $\hat{F}\varphi_\uparrow(\vec{k}) = \varphi_\downarrow(-\vec{k})$ and $\hat{F}\varphi_\downarrow(\vec{k}) = \varphi_\uparrow(-\vec{k})$.
Action of inversion: $\hat{I}\phi_\sigma(\vec{k}) = \phi_\sigma(-\vec{k})$, $\sigma = \{\uparrow, \downarrow\}$.
Check combined action: $\hat{F}\hat{I}\varphi_\uparrow(\vec{k}) \stackrel{?}{=} \varphi_\downarrow(\vec{k})$.
True → Antiferromagnet: spin-up and spin-down bands are degenerate.
Note: inversion center is located in the midpoint between spin-up and spin-down sites.
False → Altermagnet: inversion mapping spin-up to spin-down sublattice is absent.

Example

```
$ amcheck.py Mn3Fe.cif Mn3Fe.cif
============================================================
Processing: Mn3Fe.cif
------------------------------------------------------------
Spacegroup: P6_3/mmc (194)
Writing the used structure to auxiliary file:
check Mn3Fe.cif_amcheck.vasp.
Orbit of Mn atoms at positions:
1 (1) [0.156793 0.313586 0.75    ]
2 (2) [0.843207 0.686414 0.25    ]
3 (3) [0.686414 0.843207 0.75    ]
4 (4) [0.313586 0.156793 0.25    ]
5 (5) [0.156793 0.843207 0.75    ]
6 (6) [0.843207 0.156793 0.25    ]
Type spin (u, U, d, D, n, N, nn or NN) for each of them
(space separated):
u d u d u d
Orbit of Fe atoms at positions:
7 (1) [0.333333 0.666667 0.25    ]
8 (2) [0.666667 0.333333 0.75    ]
Type spin (u, U, d, D, n, N, nn or NN) for each of them
(space separated):
u d
Altermagnet? False
============================================================
Processing: Mn3Fe.cif
------------------------------------------------------------
Spacegroup: P6_3/mmc (194)
Writing the used structure to auxiliary file:
check Mn3Fe.cif_amcheck.vasp.
Orbit of Mn atoms at positions:
1 (1) [0.156793 0.313586 0.75    ]
2 (2) [0.843207 0.686414 0.25    ]
3 (3) [0.686414 0.843207 0.75    ]
4 (4) [0.313586 0.156793 0.25    ]
5 (5) [0.156793 0.843207 0.75    ]
6 (6) [0.843207 0.156793 0.25    ]
Type spin (u, U, d, D, n, N, nn or NN) for each of them
(space separated):
u u u d d d
Orbit of Fe atoms at positions:
7 (1) [0.333333 0.666667 0.25    ]
8 (2) [0.666667 0.333333 0.75    ]
Type spin (u, U, d, D, n, N, nn or NN) for each of them
(space separated):
u d
Altermagnet? True
```

https://github.com/amchecker/amcheck

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