Magnetic anisotropy in frustrated clusters and monolayers: Cr on triangular Au(111) surface

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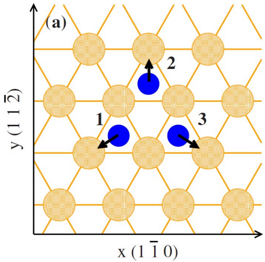
1. Introduction
2. Geometry
3. Motivation
4. Results
5. Conclusion

Frustration: basics. AFM trimer



Antal *et. al.*, PRB **77** 174429 (2008)

- Most simple Heisenberg model of a trimer:

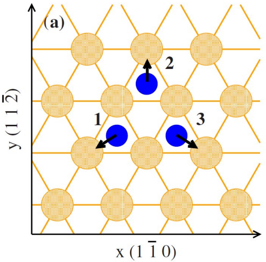
$$\mathcal{H} = J\left(\vec{\sigma}_1\vec{\sigma}_2 + \vec{\sigma}_2\vec{\sigma}_3 + \vec{\sigma}_3\vec{\sigma}_1\right) =$$
$$= \frac{1}{2}J\underbrace{\left(\vec{\sigma}_1 + \vec{\sigma}_2 + \vec{\sigma}_3\right)^2}_{0\le\quad\le 3^2} - \frac{3}{2}J$$

When $J > 0$ (antiferromagnet) the ground state is: $\vec{\sigma}_1 + \vec{\sigma}_2 + \vec{\sigma}_3 = 0$.

- Heisenberg model of a trimer up to 2nd order:

$$\mathcal{H} = \frac{1}{2}\sum_{i\neq j} J_{ij}\vec{\sigma}_i\vec{\sigma}_j$$
$$+\frac{1}{2}\sum_{i\neq j}\vec{\sigma}_i \underline{\underline{J}}^S_{ij}\vec{\sigma}_j + \frac{1}{2}\sum_{i\neq j}\vec{D}_{ij}\cdot\left(\vec{\sigma}_i\times\vec{\sigma}_j\right)$$
$$+\sum_i \vec{\sigma}_i\underline{\underline{K}}_i\vec{\sigma}_i$$

Frustration: basics. AFM trimer



Antal *et. al.*, PRB **77** 174429 (2008)

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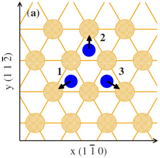
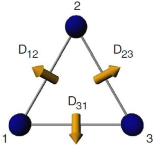
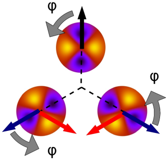
Frustration: AFM trimer





Antal *et. al.*, PRB **77** 174429 (2008)



- Heisenberg model of a trimer up to 2nd order:

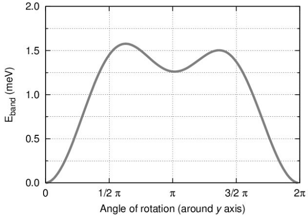
$$\mathcal{H} = \frac{1}{2}\sum_{i\neq j} J_{ij}\vec{\sigma}_i\vec{\sigma}_j + \frac{1}{2}\sum_{i\neq j}\vec{\sigma}_i \underline{\underline{J}}^S_{ij}\vec{\sigma}_j + \frac{1}{2}\sum_{i\neq j}\vec{D}_{ij}\cdot(\vec{\sigma}_i\times\vec{\sigma}_j) + \sum_i \vec{\sigma}_i\underline{\underline{K}}_i\vec{\sigma}_i$$

- Taking into account the
  - C_{3v} symmetry and
  - $\vec{\sigma}_1+\vec{\sigma}_2+\vec{\sigma}_3=0$:

$$\mathcal{H} = \vec{D}_{12}(\vec{\sigma}_1\times\vec{\sigma}_2) + \vec{D}_{23}(\vec{\sigma}_2\times\vec{\sigma}_3) + \vec{D}_{31}(\vec{\sigma}_3\times\vec{\sigma}_1) + + K^{zz}\left((\sigma_1^z)^2 + (\sigma_2^z)^2 + (\sigma_3^z)^2\right) + + K^{\varphi}\left(\cos(2\varphi_1) + \cos(2\varphi_2) + \cos(2\varphi_3)\right)$$

Results (in advance): roty

Rotating the whole spin configuration around the y axis:



different chirality states:
at $\theta = 0$ and at $\theta = \pi$.

$$\Delta E = 1.26\,\mathrm{meV}$$

Present work

$$\vec{\kappa} \overset{\text{Def.}}{=} \frac{2}{3\sqrt{3}} \sum_{ij=12,23,31} (\vec{\sigma}_i \times \vec{\sigma}_j)$$

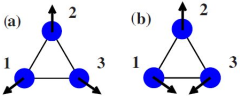


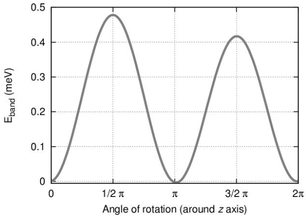
FIG. 5. (Color online) Two typical ground state configurations of an equilateral Cr trimer in the absence of DM interactions. The two configurations refer to different chiralities: (a) $\kappa_z = -1$ and (b) $\kappa_z = 1$; see Eq. (21).

$$\Delta E = 5.04\,\mathrm{meV}$$

Antal *et. al.*, PRB **77** 174429 (2008)

Results (in advance): rotz

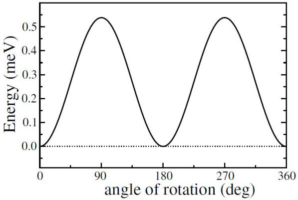
Rotating the whole spin configuration around the z axis:



$$K^{\varphi} = 75\ \mu\text{eV}$$

(amplitude: $6K^{\varphi}$)

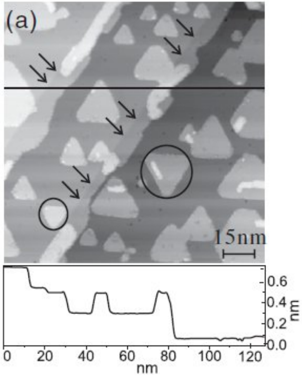
Present work

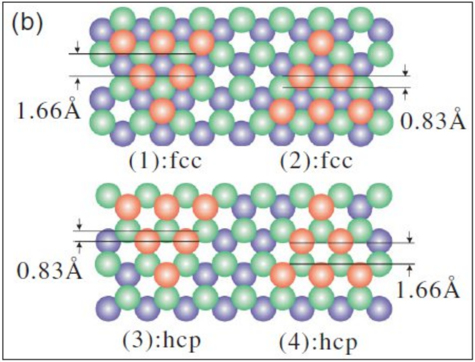


$$K^{\varphi} \approx 90\ \mu\text{eV}$$

Stocks *et. al.*, Prog. Mat. Sci. **52** 371–387 (2007)

SP-STM Experiment: Mn islands on Ag(111) (Gao *et. al.* (2008))



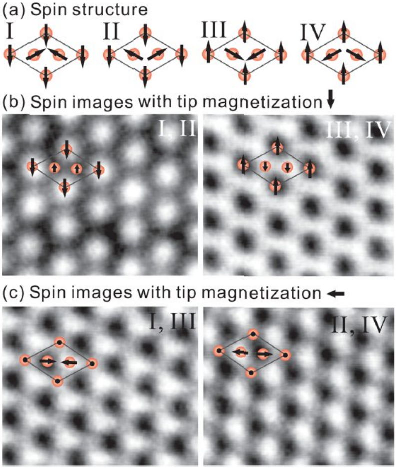


(a) Topography of 0.6 monolayer Mn on Ag(111).

(b) Red: Mn atoms;
green and blue: first and second Ag layer
ABCABCAB|C stacking: **fcc**
ABCABCAB|A stacking: **hcp**

Gao *et. al.*, PRL **101** 267205 (2008)

SP-STM Experiment: Mn islands on Ag(111) (Gao *et. al.* (2008))



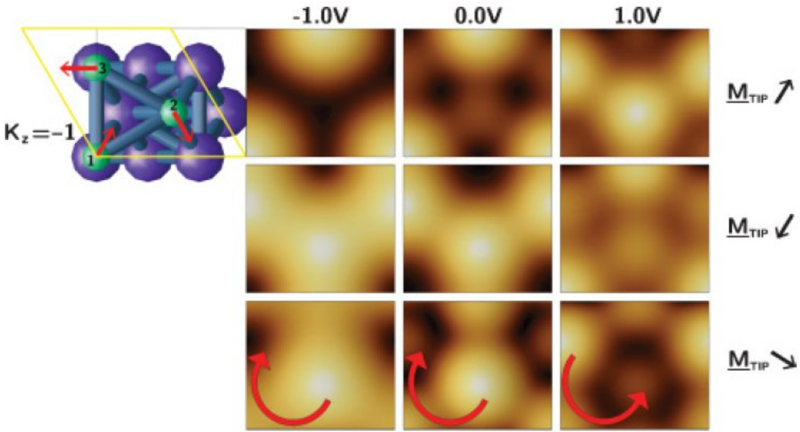
SP-STM images taken on *up* islands.

They concluded that 120° Néel structure was observed on both *up* and *down* islands but with different orientation of the individual moments.

'A disagreement with the previous theoretical predictions indicates that a careful reinvestigation is needed in theory.'

Gao *et. al.*, PRL **101** 267205 (2008)

Comment by Krisztián Palotás

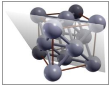


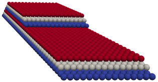
They *'showed evidence that the magnetic contrast is sensitive to the tip electronic structure, and this contrast can be reversed depending on the bias voltage.'*

Palotás *et. al.*, PRB **84** 174428 (2011)

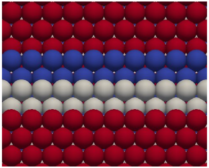
Trimer positions on fcc(111) triangular surface

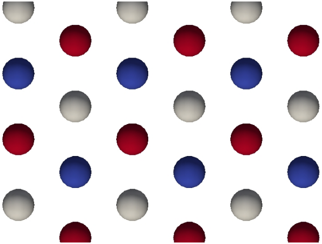
ABCABC|A stacking: **fcc**
ABCABC|B stacking: **hcp**





http://www.xcrysden.org/img/rh_fcc_111plane-200.png

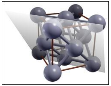


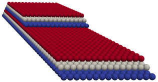


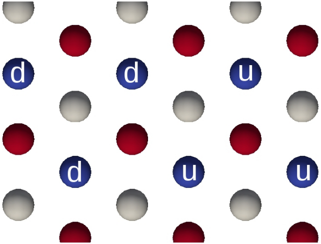
- top Au layer: red
- fcc substrate pos.: above the blue Au layer
- hcp substrate pos.: above the grey Au layer

Trimer positions on fcc(111) triangular surface

ABCABC|A stacking: **fcc**
ABCABC|B stacking: **hcp**







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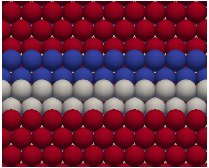
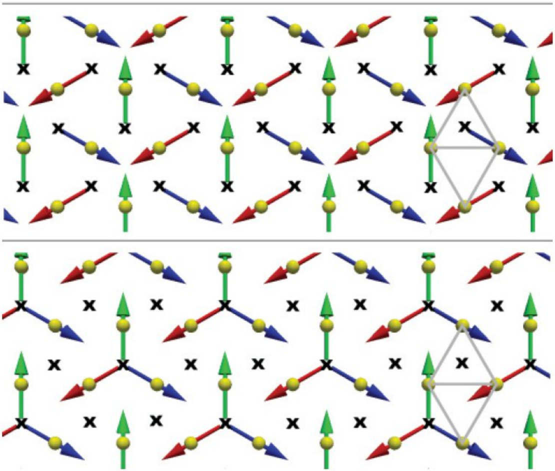


- top Au layer: red
- fcc substrate pos.: above the blue Au layer
- hcp substrate pos.: above the grey Au layer
- fcc trimer positions: *up* (u) or *down* (d)
- hcp trimer positions: also *up* or *down*

Monolayer positions on fcc(111) triangular surface



dos Santos Dias *et. al.*, PRB **83** 054435 (2011)

Motivation

The aim of the present work is...

- to perform a complete investigation of the ground state of...
- determine the coefficients in the Heisenberg model for...

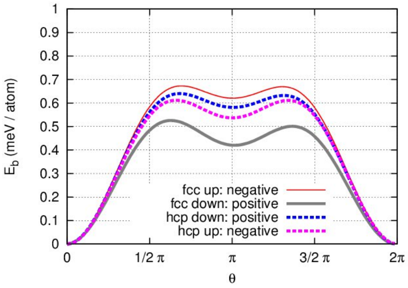
All trimers:

$$\{\textbf{fcc}, \textbf{hcp}\} \otimes \{\textbf{up}, \textbf{down}\} \otimes \{\boldsymbol{\kappa}^+, \boldsymbol{\kappa}^-\}$$

All monolayers:

$$\{\textbf{fcc}, \text{hcp}\} \otimes \{\boldsymbol{\kappa}^+, \boldsymbol{\kappa}^-\}$$

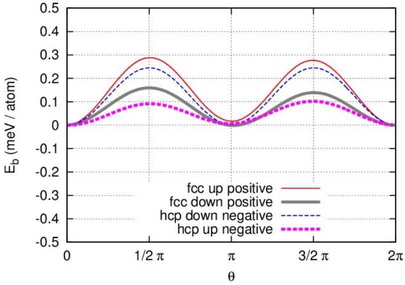
Trimers' chiral anisotropy: roty



Note: $\theta = 0$ or π always refer to opposite chiralities.

Trimers' in-plane anisotropy: rotz

- In-plane anisotropy in one chirality states of the 4 trimers:



- The in-plane anisotropy vanishes ($< 3\,\mu$eV/atom) in the other chirality states. **Why?**

Trimers' in-plane anisotropy: rotz

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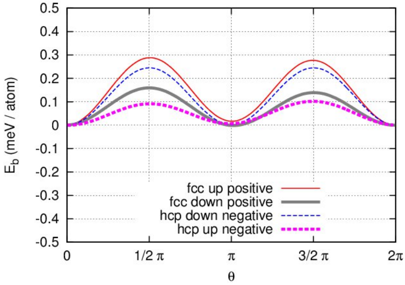

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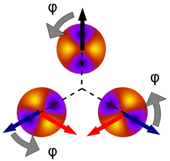
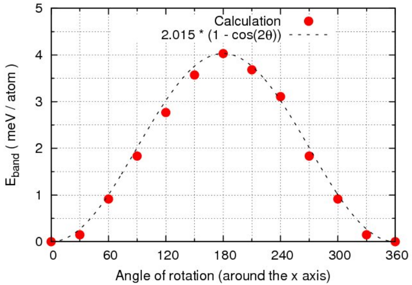


- $-3\cos(2\phi)$
- $-\cos(2\phi) - \cos(2\phi + 120^\circ) - \cos(2\phi + 240^\circ) = 0$

FCC monolayer's anisotropy

- Chiral anisotropy:



- **Interesting:** the two different chirality monolayers can be distinguished energetically. The magnetic unit cell of the monolayer can be considered as 1 up trimer + 1 down trimer.
- The in-plane anisotropy $< 0.1\,\mu\text{eV}/\text{atom}$.
- It is OK: the monolayer has higher symmetry, a $K^{\varphi}\cos(2\varphi)$ on-site anisotropy term has to vanish.

HCP monolayer's anisotropy

Remaining work. . .

Values (μeV/atom)

On-site uniaxial (K^{zz}):

	up	down	monolayer
fcc	91	87	?
hcp	93	89	

Chiral (D^{z}):

	up	down	monolayer
fcc	120	81	776
hcp	104	112	

In-plane (K^{φ}):

	up	down	monolayer
fcc	46	25	$=0$
hcp	16	41	$=0$

Conclusions

Trimers $(\{\mathrm{fcc}, \mathrm{hcp}\} \otimes \{\mathrm{up}, \mathrm{down}\} \otimes \{\kappa^+, \kappa^-\})$

- We could calculated: ground state & anisotropy terms in a 2^{nd} order Heisenberg model.
- We state that experimentally undistinguisable trimers exhibit similar magnetic behaviour therefore the position with respect to the topmost Au layer is important.

FCC monolayer

- The ground state and the anisotropy terms are also accessible.
- A monolayer can be considered to be built of trimers as 'bricks'.

Remaining work...

- hcp monolayer

Bonus

Suggested article: *Chirality of Triangular Antiferromagnetic Clusters as a Qubit*, Georgeot and Mila, PRL **104** 200502 (2010)

- Chirality of a Cu trimer is proposed to be used as a qubit
- Representation of the qubit: scalar chirality:

$$\vec{S}_1 \cdot \left(\vec{S}_2 \times \vec{S}_3 \right)$$

  $\vec{S}_i$: quantum 1/2 spin operators

- One-qubit rotations: tuning the exchange coupling inside the triangles (J) with an STM tip
- CNOT gate: tuning the exchange interaction between neighbouring triangles (J') with an STM tip