# Magnetic anisotropy in deposited Cr clusters

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Turku, Finnland, 15–17 February 2012

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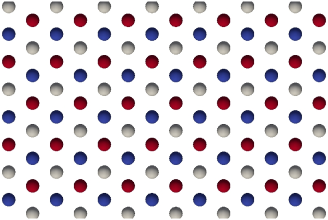
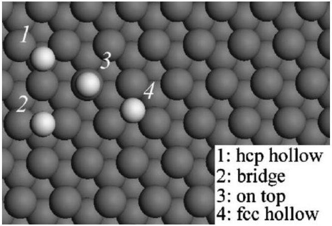
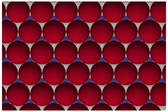
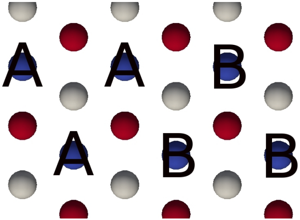
# The (111) surface of fcc Au

TOP + 1
TOP
TOP – 1
TOP – 2








H. J. Gotsis *et al.*, Phys. Rev. B **73,** 014436 (2006)

Without intralayer relaxation, there are 8 different cluster positions for a compact trimer.

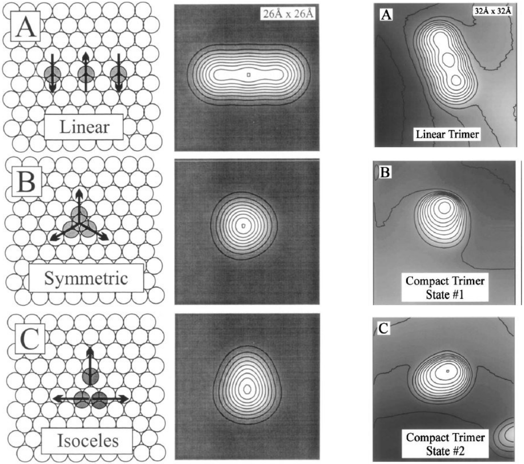
# Frustration

Most simple classical vector spin model for 3 spins: (isotropic Heisenberg model)

$$\mathcal{H} = J\left(\boldsymbol{\sigma}_1\boldsymbol{\sigma}_2 + \boldsymbol{\sigma}_2\boldsymbol{\sigma}_3 + \boldsymbol{\sigma}_3\boldsymbol{\sigma}_1\right)$$
$$= \frac{1}{2}J\left(\boldsymbol{\sigma}_1 + \boldsymbol{\sigma}_2 + \boldsymbol{\sigma}_3\right)^2 - \frac{3}{2}J$$

- Ferromagnetic: $\boldsymbol{\sigma}_1 \parallel \boldsymbol{\sigma}_2 \parallel \boldsymbol{\sigma}_3$, collinear ground state
- Antiferromagnetic: $\boldsymbol{\sigma}_1 + \boldsymbol{\sigma}_2 + \boldsymbol{\sigma}_3 = \mathbf{0}$, planar, non-collinear ground state, $\measuredangle(\boldsymbol{\sigma}_i, \boldsymbol{\sigma}_j) = 120^\circ$

# Fabricating and analyzing Cr trimers with STM

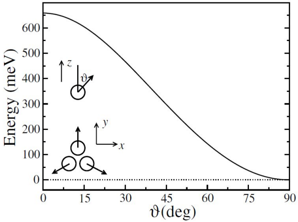


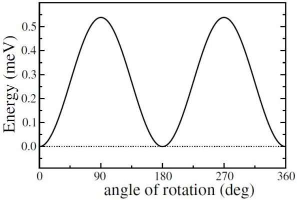

Conditions: $T = 7\,\mathrm{K}$, ultrahigh vacuum, resolution $\approx 5\,\text{Å}$. Measuring STM $\mathrm{d}I/\mathrm{d}V$ spectra on the trimers, they experienced two different kinds of curves: one without any resonance at the Fermi energy, and another showing a Fano shape resonance with a Kondo temperature of $T_\mathrm{K} = 50 \pm 10\,\mathrm{K}$.

S. Uzdin *et al.*, Europhys. Lett. **47,** 556 (1999)
T. Jamneala *et al.*, Phy. Rev. Lett. **87,** 256804 (2001)

# *Ab-inito* spin-dynamics; magnetic force theorem (MFT)

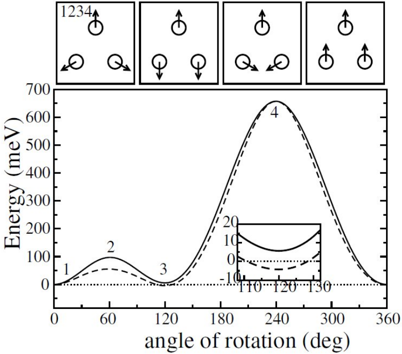
- From damped *ab-initio* spin dynamics, G. M. Stocks *et al.* found an in-plane 120° Néel strucure as ground state
- It was hard to determine the orientation with respect to the crystal, however, possible
- $J = 146.7\,\text{meV}$




G. M. Stocks *et al.*, Prog. Mat. Sci. **52,** 371 (2007)

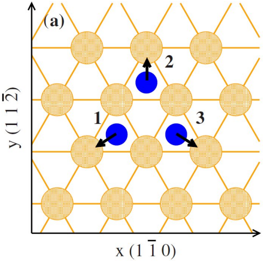
# Magnetic force theorem (MFT)




- The energy difference between the different chirality states (1, 3) is +7 meV or –4 meV, *depending on the self-consistent potential*

G. M. Stocks *et al.*, Prog. Mat. Sci. **52,** 371 (2007)

# Least square fit of a model Hamiltonian




A. Antal *et al.*, Phys. Rev. B **77,** 174429 (2008)

$$\mathcal{H} = \frac{1}{2}\sum_{i\neq j} J_{ij}\boldsymbol{\sigma}_i\boldsymbol{\sigma}_j + \frac{1}{2}\sum_{i\neq j}\boldsymbol{\sigma}_i\mathbf{J}^{S}_{ij}\boldsymbol{\sigma}_j + \frac{1}{2}\sum_{i\neq j}\mathbf{D}_{ij}\cdot(\boldsymbol{\sigma}_i\times\boldsymbol{\sigma}_j) + \sum_i \boldsymbol{\sigma}_i\mathbf{K}_i\boldsymbol{\sigma}_i + Q\Big[(12)^2+(13)^2+(23)^3\Big] + 2Q'\Big[(12)(13)+(21)(23)+(31)(32)\Big]$$

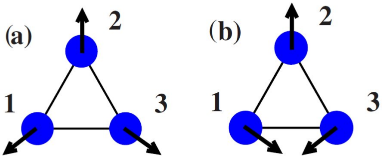
For the above Hamiltonian, the Landau–Lifshitz–Gilbert equation is solved to determine the ground state.

# Chirality. Results of A. Antal *et al.*

For in-plane configurations:

$$E_{\mathrm{DM}} = \frac{1}{2}\sum_{i\neq j} \mathbf{D}_{ij} \cdot (\boldsymbol{\sigma}_i \times \boldsymbol{\sigma}_j) = \frac{3\sqrt{3}}{2} D_z \kappa_z,$$

where $\boldsymbol{\kappa} = \frac{2}{3\sqrt{3}} \sum_{(ij)} \boldsymbol{\sigma}_i \times \boldsymbol{\sigma}_j$ is the *chirality vector* of the trimer.

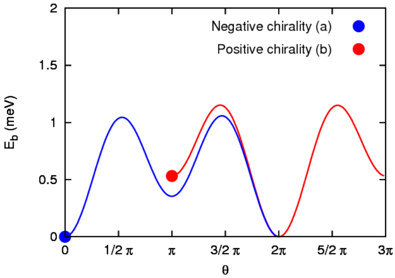


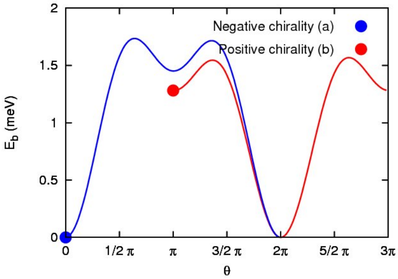

There is an energy difference of $\Delta E = 5.04\,\mathrm{meV}$ between the two different chirality states. Ground state: **(a)**, $\kappa_z = -1$.

A. Antal *et al.*, Phys. Rev. B **77,** 174429 (2008)

# Global rotation around the $y$ axis: MFT band energy

- All magnetic moments were rotated simultaneously around the $y$ axis

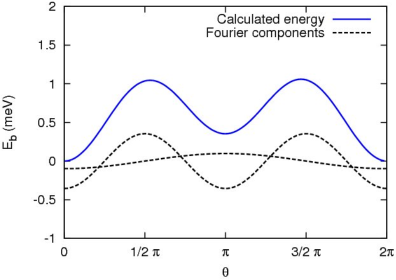


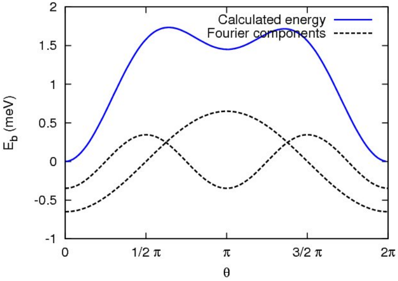




- The calculated energy differences are $\approx 0.4\,\mathrm{meV}$ ($\approx 4.5\,\mathrm{K} \cdot k_\mathrm{B}$) and $\approx 1.3\,\mathrm{meV}$ ($\approx 15\,\mathrm{K} \cdot k_\mathrm{B}$) for the two clusters
- These value do not coincide with the result of A. Antal *et al.*, however, the nearest neighbors were also included in our calculation

# Global rotation around the $y$ axis: MFT band energy

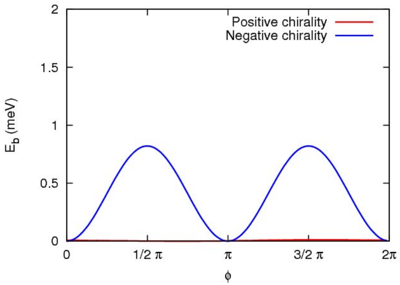
- The Fourier components of the energy function are calculated

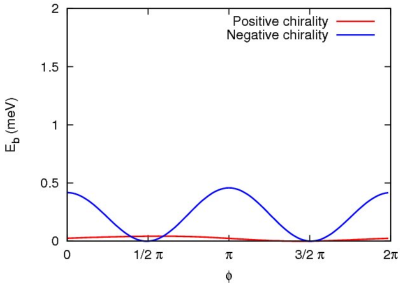


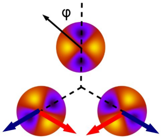

- From the uniaxial on-site anisotropy: $\cos(2\theta)$
- From the DM interaction: $\cos(\theta)$

# Global rotation around the $z$ axis: MFT band energy




- Why does the chirality “kill” the anisotropy?




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

# $2^{\text{nd}}$ order in-plane anisotropy

Fixing all spins exept one, and expanding the energy function in terms of real spherical harmonics. [meV]

| In-plane anis. function | adatom | A+ | A– | B+ | B– |
|---|---|---|---|---|---|
| $\frac{1}{2}\sqrt{\frac{15}{\pi}}\,xy$ | 0 | 2.59 | –2.76 | 5.86 | –5.59 |
| $\frac{1}{4}\sqrt{\frac{15}{\pi}}(x^2-y^2)$ | 0 | 1.49 | 1.60 | 3.37 | 3.49 |

# Summary, future plans

## Summary

- A literature overview on $Cr_3$ clusters is presented
- The presented results fit in the previous works

## Future plans

- Investigating the rest of the 16 clusters (*fcc hollow*, hcp hollow, bridge, on top; $\kappa_z > 0$, $\kappa_z < 0$)
- Try to find the ground state with a new idea based on the Newton–Raphson method

**Thank you for your attention**