

# Novel Monte Carlo study of deposited magnetic nanoparticles

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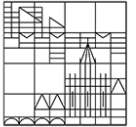
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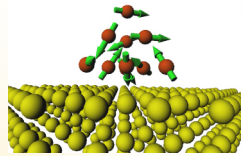
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## Introduction

- In order to study the finite temperature behavior of magnetic nanoparticles, a novel Monte Carlo method has been developed. The energy of a new trial configuration during the simulation is calculated directly from the expansion of the band energy avoiding the set up of an *a priori* Heisenberg-type model.
- Studies of deposited magnetic nanoparticles



magnetic cluster,  
e.g., Cr, Co

non-magnetic (semi-infinite) host,  
e.g., Au(111), Cu(001)

- The magnetic properties of a wide class of systems are often described by the classical Heisenberg model,

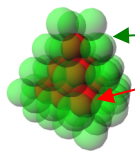
$$\mathcal{H} = \frac{1}{2} \sum_{i,j} J_{ij} \sigma_i \sigma_j - \sum_i K (\sigma_i^z)^2,$$

where isotropic coupling between spins and uniaxial anisotropy are considered. We compare the *ab initio* and the Heisenberg model based temperature dependence of the magnetic moment of a  $\text{Co}_{4 \times 4} \text{Cu}(001)$  cluster, and find good agreement for this particular case.

## Computational method I. – Electronic structure

- Electronic structure calculation: fully relativistic implementation of the local spin-density approximation of the density functional theory
- Embedded cluster Green's function technique based on the KKR method [1]

$$\tau(\varepsilon) = \tau_{\text{host}}(\varepsilon) \left( \mathbf{I} - \Delta \mathbf{t}^{-1}(\varepsilon) \tau_{\text{host}}(\varepsilon) \right)^{-1}$$



environment (vacuum or host atoms)

real cluster (e.g., Cr or Co atoms)

- Self-consistent cluster calculation

- then: frozen potential approximation

- Taylor-expansion of the band energy:

$$E_b \approx E_0 + \sum_{i=1}^N \frac{\partial E_b}{\partial \sigma_i} \Big|_{\{\sigma_0\}} \Delta \sigma_i + \frac{1}{2} \sum_{i,j=1}^N \Delta \sigma_i^T \frac{\partial^2 E_b}{\partial \sigma_i \partial \sigma_j} \Big|_{\{\sigma_0\}} \Delta \sigma_j$$

- The derivatives of the band energy can be calculated analytically from Lloyd's formula, see [2].

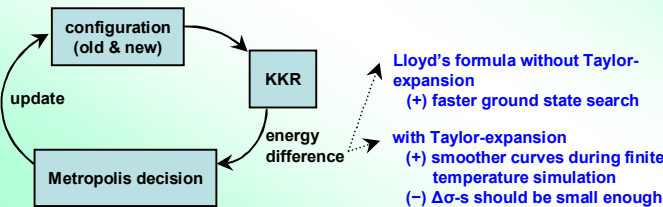
$$E_b = -\frac{1}{\pi} \text{Im} \int_{-\infty}^{\varepsilon_F} \text{Tr} \ln \tau(\varepsilon) d\varepsilon$$

## Computational method II. – Monte Carlo simulation

- Ground state by simulated annealing
- Finite temperature simulation
- We used the Metropolis algorithm with single spin flip dynamics:

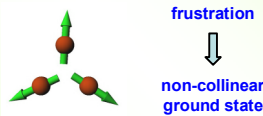
$$P(i \rightarrow f) = \begin{cases} 1, & \text{if } E_f \leq E_i, \\ e^{-\beta(E_f - E_i)}, & \text{if } E_f > E_i. \end{cases}$$

- Flowchart of the code:

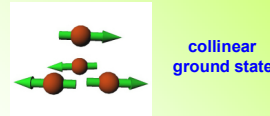


## Results I. – Ground state of AFM and FM clusters

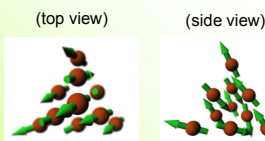
- Benchmark system: Cr trimer on Au(111) surface. The same ground state was found in [3] by solving the Landau–Lifshitz–Gilbert equations.



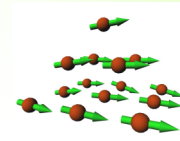
- Tetrahedron shaped Cr particle on Au(111) surface. Similar ground state was found in [4] for the same Cr cluster on Cu(111) surface.



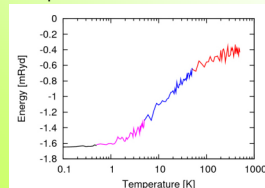
- Ground state of a pyramid shaped  $\text{Cr}_{10}$  cluster on Au(111) surface



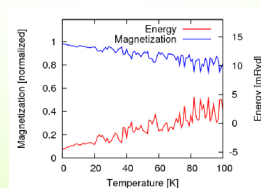
- Ground state of a pyramid shaped  $\text{Co}_{14}$  cluster on Cu(001) surface



- Simulated annealing of this cluster in four steps

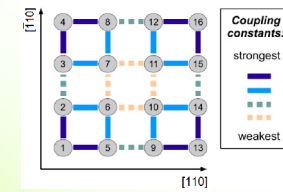


- Simulated annealing of this cluster



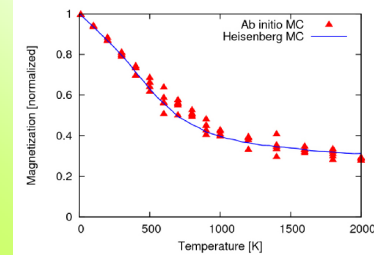
## Results II. – Thermodynamics of a $\text{Co}_{4 \times 4} \text{Cu}(001)$ cluster

- Geometry and isotropic coupling constants between next nearest neighbors



Coupling constants	[mRyd]	Magnetic moments	[ $\mu_B$ ]
$J_{1-5}$	5.59	$m_1$	1.74
$J_{5-6}$	5.27	$m_5$	1.82
$J_{5-9}$	4.49	$m_6$	1.87
$J_{6-10}$	4.19		
$J_{\text{mono-layer}}$	4.26	$m_{\text{mono-layer}}$	1.88

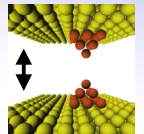
- Square root of the thermal average of the square of the magnetization:



- In the Heisenberg MC simulation, we used  $10^5$  MC steps per temperature points and the anisotropy constant of the monolayer cobalt on Cu(001) surface,  $K = 0.0228$  mRyd;
- in the *ab initio* MC simulation we used  $5 \times 10^4$  MC steps per temperature points.

## Future plans

- Simulating an "STM tip" and investigating the distance-dependence of its magnetic structure and ground state



- Further studies of the thermodynamics of magnetic nanoparticles (magnetic switching)

## References and acknowledgments

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