MŰEGYETEM 1782

Theoretical study of a domain wall through a cobalt nano-contact

László Balogh, Krisztián Palotás, Bence Lazarovits,
László Udvardi, László Szunyogh

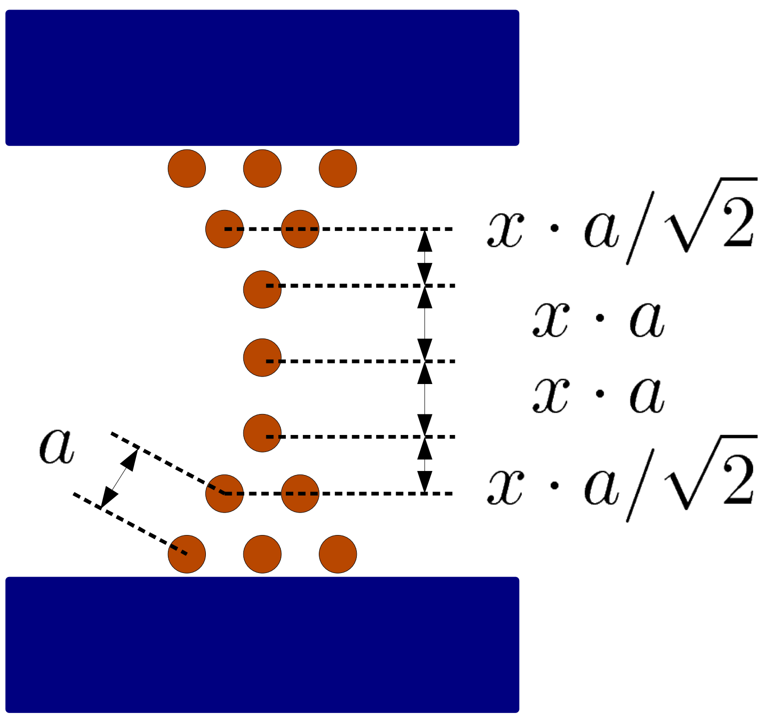
Sovata, June 1—4, 2011.

Contents

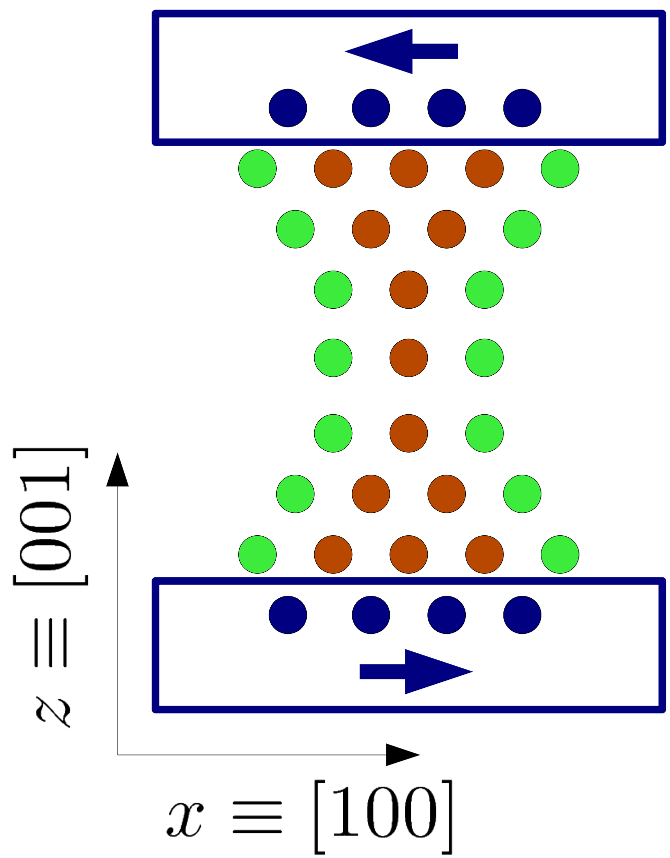
- Structure of the contact
- Modeling methods
- Relativistic effects
  - rotation around the [100] axis
  - decomposition of the band energy (E_b) on the central atom

Physical system:

Co[001] + 3 x 3 + 2 x 2 + 1 + 1 + 1 + 2 x 2 + 3 x 3 + Co[001]



$$x \in \{0.85, \ldots, 1.15\}$$



Isotropic Heisenberg model

$$\mathcal{H} = \frac{1}{2} \sum_{i \neq j} J_{ij} \, \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j$$

Invariant under global spin rotation.

Boundary condition: [100] and [$\bar{1}$00]

Invariant under global spin rotation around the [100] axis.

Configurations rotated around the [100] axis are equivalent.

Deficiensies of the isotropic Heisenberg model

Higher order terms can appear, *e.g.,*

$$J_{\square}\left[(\boldsymbol{\sigma}_1\boldsymbol{\sigma}_2)(\boldsymbol{\sigma}_3\boldsymbol{\sigma}_4)+(\boldsymbol{\sigma}_2\boldsymbol{\sigma}_3)(\boldsymbol{\sigma}_4\boldsymbol{\sigma}_1)+(\boldsymbol{\sigma}_1\boldsymbol{\sigma}_3)(\boldsymbol{\sigma}_2\boldsymbol{\sigma}_4)\right]$$

(see: S. Lounis, P. H. Dederichs, Phys. Rev. B. **82**, 180404 (2010))

$$\mathbf{J}_{ij}$$

$$\mathbf{J}_{ij}^{\mathrm{I}}=\left(\frac{1}{3}\mathrm{Tr}\,\mathbf{J}_{ij}\right)\mathbf{I}$$

$$\mathbf{J}_{ij}^{\mathrm{S}}=\frac{1}{2}\left(\mathbf{J}_{ij}+\mathbf{J}_{ij}^{T}\right)-\mathbf{J}_{ij}^{\mathrm{I}}$$

$$\mathbf{J}_{ij}^{\mathrm{A}}=\frac{1}{2}\left(\mathbf{J}_{ij}-\mathbf{J}_{ij}^{T}\right)$$

On-site anisotropy, *e.g.,* $K(\theta)=-K_2\sin^2(\theta)$

Demonstrations of the relativistic effects:

♣ ***energy while rotating the whole configuration around the [100] axis.***

♣ ***expansion of the energy of the most symmetric atom in terms of the real sperical harmonics***

Modeling methods I.

Screened Korringa–Kohn–Rostoker / embedded cluster method [1]

Infinitesimal rotations method: [2]
► parameters of isotropic Heisenberg model

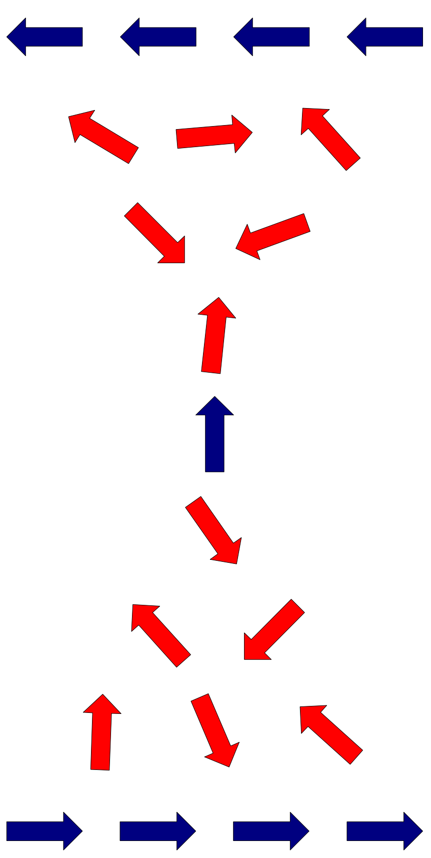
Monte Carlo: simulated annealing / Metropolis algorithm
► ≈ ground state

Minimization of the band energy by Newton−Raphson method: an iterative minimum searching algorithm
► ground state magnetic configuration
► potential (V, B_{xc}) at this configuration

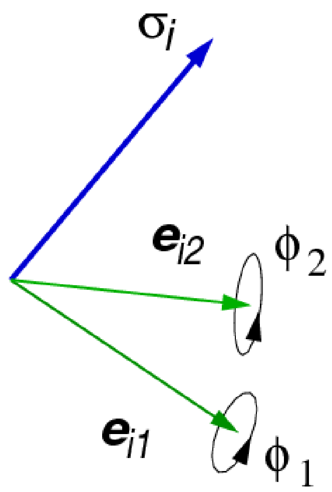
Embedding + band energy calculation + magnetic force theorem
► energy functions

[1] B. Lazarovits, *et. al.* PRB **65**, 104441 (2002)

[2] A.I. Liechtenstein *et al.* JMMM **67**, 65 (1987)
[2] L. Udvardi *et al.* PRB **68**, 104436 (2003)



Modeling methods II.

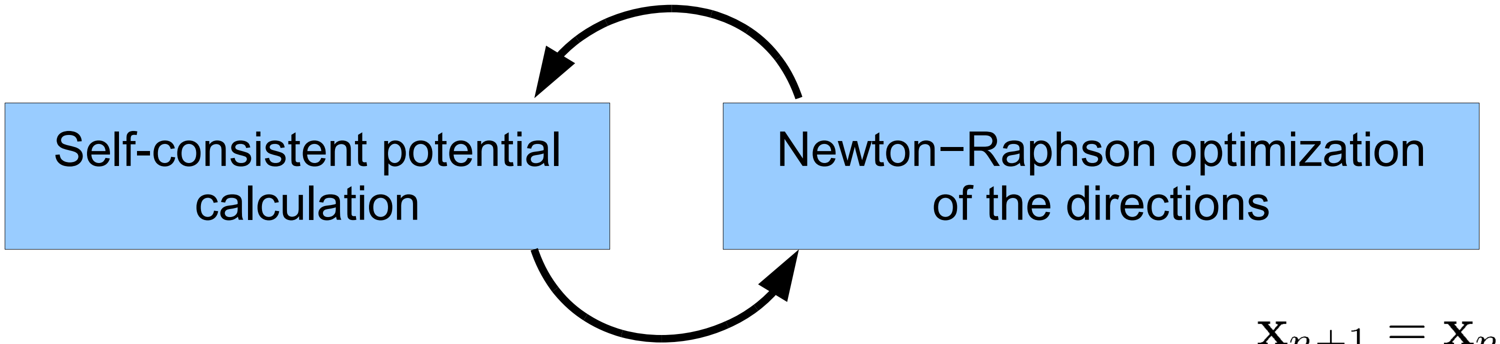


$$E_\mathrm{b} = \int_{-\infty}^{E_\mathrm{F}} (\varepsilon - E_\mathrm{F}) n(\varepsilon)\, \mathrm{d}\varepsilon = -\frac{1}{\pi} \mathrm{Im} \int_{-\infty}^{E_\mathrm{F}} \mathrm{Tr} \ln \tau(\varepsilon)\, \mathrm{d}\varepsilon$$

$$\frac{\partial E_\mathrm{b}}{\partial \phi_{i\alpha}} = \frac{1}{\pi} \mathrm{Im} \int_{-\infty}^{E_\mathrm{F}} i\, \mathrm{Tr} \left\{ \tau_{ii}(\varepsilon) \left[\mathbf{e}_{i\alpha} \cdot \mathbf{J}, t_i^{-1}(\varepsilon) \right] \right\} \mathrm{d}\varepsilon$$

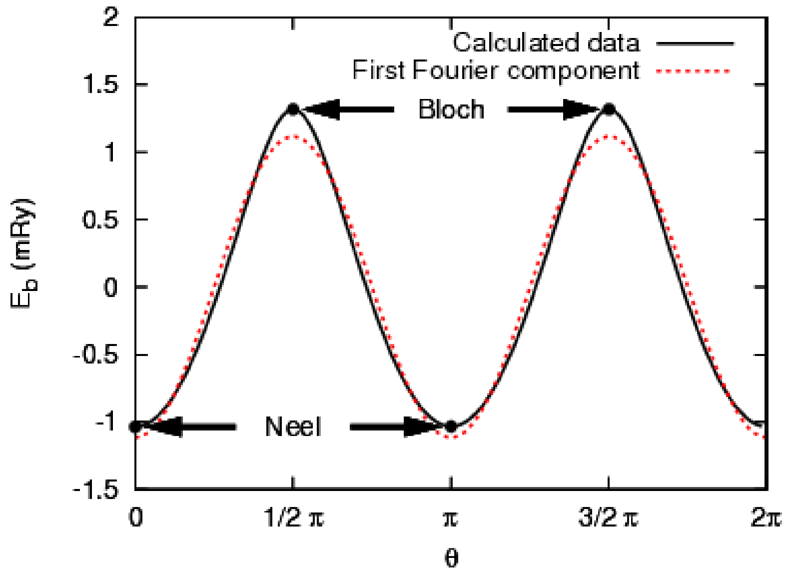
$$\frac{\partial^2 E_\mathrm{b}}{\partial \phi_{i\alpha}\, \partial \phi_{j\beta}} = \delta_{ij} \frac{1}{\pi} \mathrm{Im} \int_{-\infty}^{E_\mathrm{F}} \mathrm{Tr} \left\{ \tau_{ii}(\varepsilon) \left[\mathbf{e}_{i\alpha}\mathbf{J}, \left[\mathbf{e}_{i\beta}\mathbf{J}, t_i^{-1}(\varepsilon) \right] \right] \right\} \mathrm{d}\varepsilon$$
$$- \frac{1}{\pi} \mathrm{Im} \int_{-\infty}^{E_\mathrm{F}} \mathrm{Tr} \left\{ \tau_{ij}(\varepsilon) \left[\mathbf{e}_{j\beta}\mathbf{J}, t_j^{-1}(\varepsilon) \right] \tau_{ji}(\varepsilon) \left[\mathbf{e}_{i\alpha}\mathbf{J}, t_i^{-1}(\varepsilon) \right] \right\} \mathrm{d}\varepsilon$$

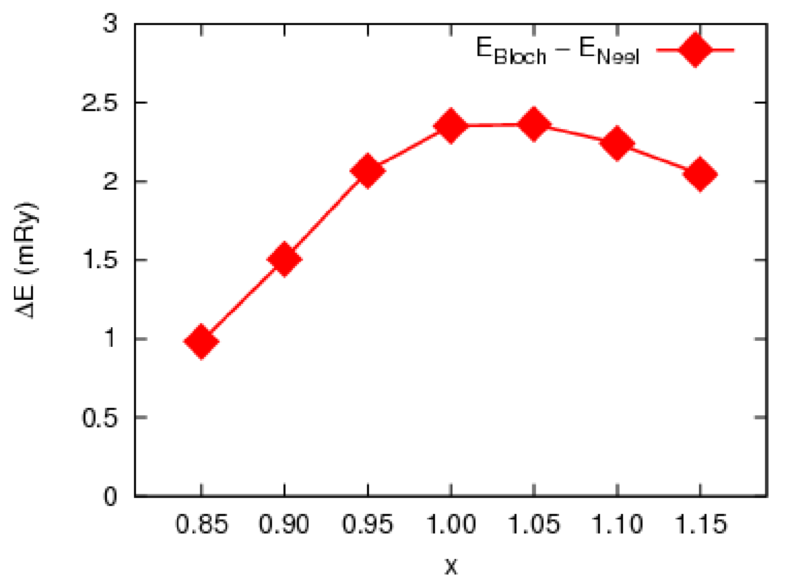
based on L. Udvardi *et al.* PRB **68**, 104436 (2003)



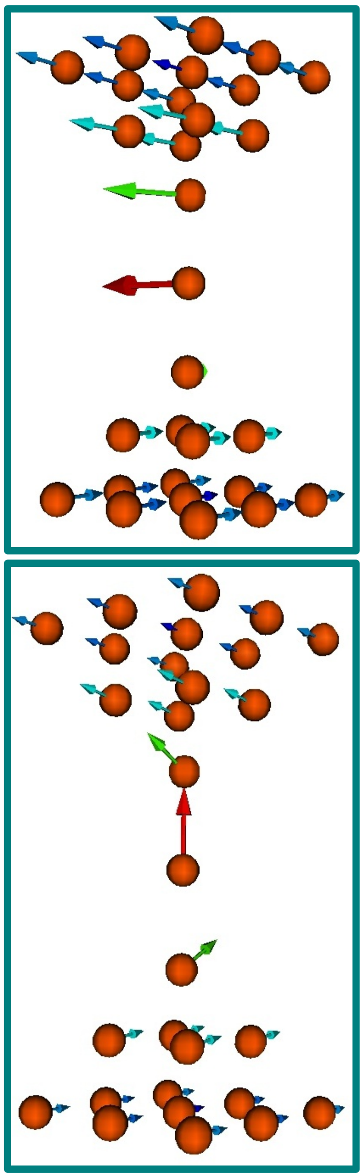
$$\mathbf{x}_{n+1} = \mathbf{x}_n - \frac{\mathrm{d}E_\mathrm{b}}{\mathrm{d}\mathbf{x}} \cdot \left(\frac{\mathrm{d}^2 E_\mathrm{b}}{\mathrm{d}\mathbf{x}^2} \right)^{-1}$$

Global spin rotation around the [100] axis I.





Bloch



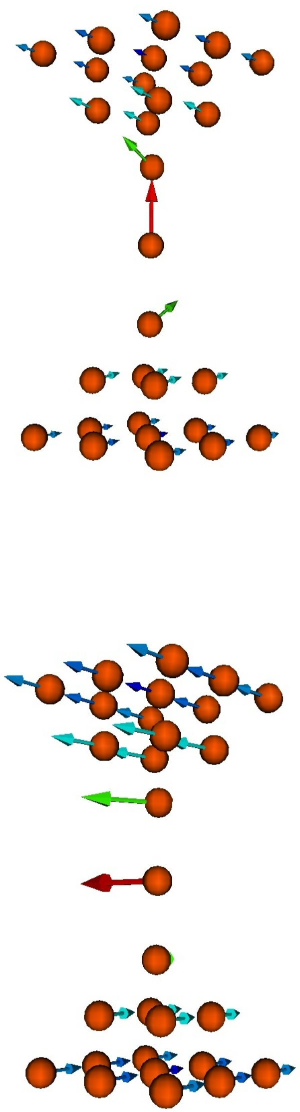
Néel

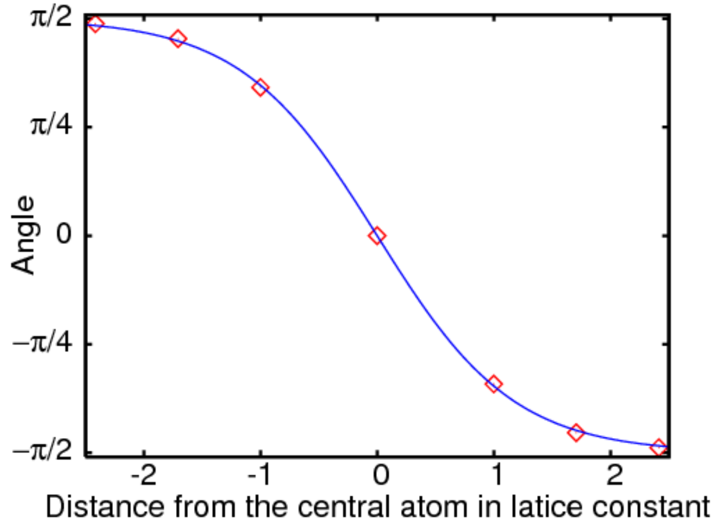
Global spin rotation around the [100] axis II.

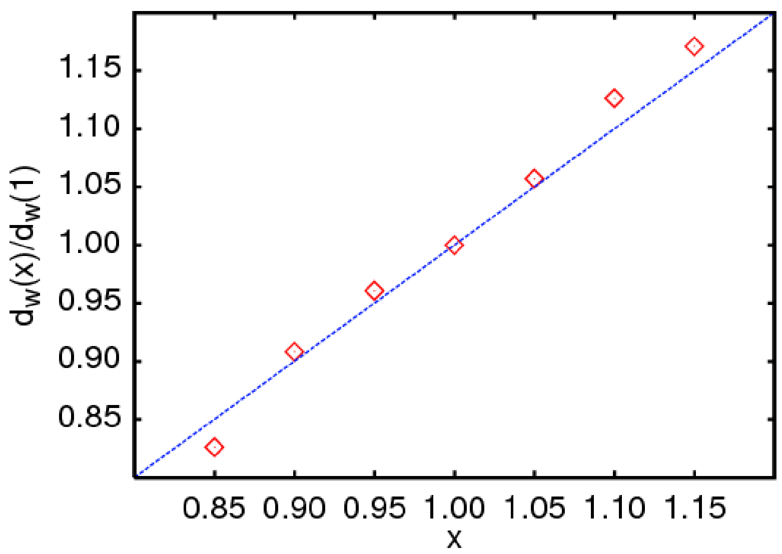
TABLE II. Fourier components of the band energy while rotating all spins around the [100] direction. The displayed coefficients are the a_k coefficients in the expansion $E_\mathrm{b} = a_0 + \sum_{k=1}^{\infty} a_k \cos(2k\theta)$. The other coefficients are practically zeros. The units are Rydberg.

x	$k=1$ ($\times 10^{-3}$ Ry)	$k=2$ ($\times 10^{-4}$ Ry)	$k=3$ ($\times 10^{-5}$ Ry)	$k=4$ ($\times 10^{-5}$ Ry)	$k=5$ ($\times 10^{-5}$ Ry)
0.85	−0.466	0.108	2.920	2.658	2.623
0.90	−0.735	0.262	3.666	2.450	2.643
0.95	−1.003	1.029	2.190	2.407	2.812
1.00	−1.116	1.594	−0.296	3.459	2.370
1.05	−1.112	1.726	−0.897	3.823	2.237
1.10	−1.055	1.644	−0.613	3.718	2.303
1.15	−0.967	1.414	0.185	3.402	2.463

Domain wall width



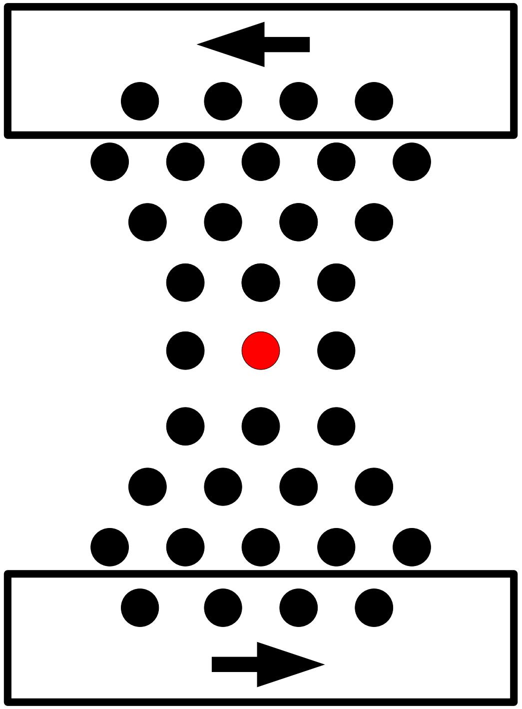




$$\varphi(z) = -\frac{\pi}{2}\mathrm{th}\left(\frac{z}{2d_{\mathrm{w}}}\right)$$

Model of the energy function I.

$$E_{\text{band}}(\underbrace{\ldots}_{\text{fixed}},\ \vartheta,\ \varphi,\ \underbrace{\ldots}_{\text{fixed}}) = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} E_{lm} Y_{lm}(\vartheta, \varphi)$$



Model of the energy function II.

$$E_{\text{band}}(\underbrace{\ldots}_{\text{fixed}}, \vartheta, \varphi, \underbrace{\ldots}_{\text{fixed}}) = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} E_{lm} Y_{lm}(\vartheta, \varphi)$$

l	
1	$\frac{1}{2}\sqrt{\frac{3}{\pi}}z$
2	$\frac{1}{4}\sqrt{\frac{5}{\pi}}\left(3z^2-1\right)$
	$\frac{1}{4}\sqrt{\frac{15}{\pi}}\left(x^2-y^2\right)$
3	$\frac{1}{4}\sqrt{\frac{7}{\pi}}\left(5z^3-3z\right)$
	$\frac{1}{4}\sqrt{\frac{105}{\pi}}\left(x^2-y^2\right)z$
4	$\frac{3}{16}\sqrt{\frac{1}{\pi}}\left(35z^4-30z^2+3\right)$
	$\frac{3}{8}\sqrt{\frac{5}{\pi}}\left(x^2-y^2\right)\left(7z^2-1\right)$
	$\frac{3}{16}\sqrt{\frac{35}{\pi}}\left(x^4-6x^2y^2+y^4\right)$

$x = 1.00$
$-1.56 \cdot 10^{-2}$
$-2.38 \cdot 10^{-3}$
$3.75 \cdot 10^{-5}$
$5.22 \cdot 10^{-5}$
$7.91 \cdot 10^{-6}$
$3.63 \cdot 10^{-4}$
$7.96 \cdot 10^{-6}$
$-2.98 \cdot 10^{-6}$

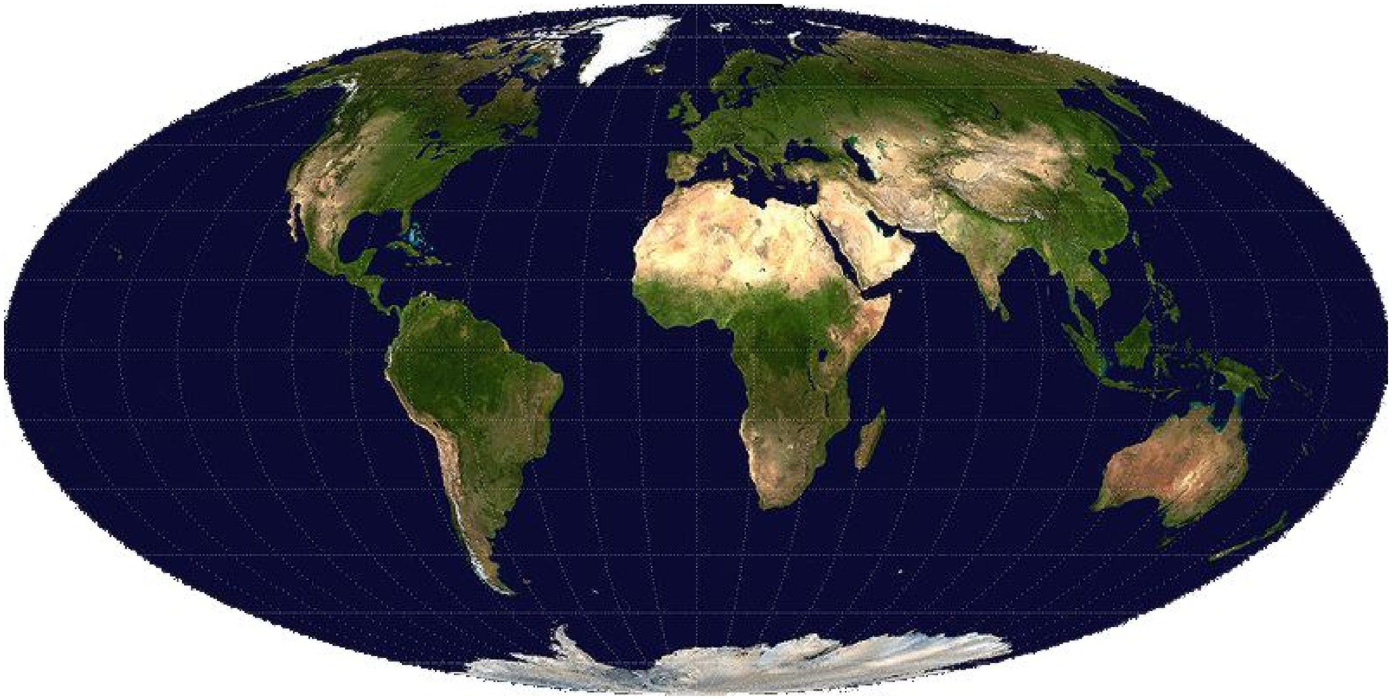
Model of the energy function III.

$$E_{\text{band}}(\underbrace{\ldots}_{\text{fixed}},\ \vartheta,\ \varphi,\ \underbrace{\ldots}_{\text{fixed}}) = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} E_{lm} Y_{lm}(\vartheta, \varphi)$$

l		$x = 0.85$	$x = 0.90$	$x = 0.95$	$x = 1.00$	$x = 1.05$	$x = 1.10$	$x = 1.15$
1	$\frac{1}{2}\sqrt{\frac{3}{\pi}}z$	$-1.77 \cdot 10^{-2}$	$-1.81 \cdot 10^{-2}$	$-1.73 \cdot 10^{-2}$	$-1.56 \cdot 10^{-2}$	$-1.41 \cdot 10^{-2}$	$-1.29 \cdot 10^{-2}$	$-1.17 \cdot 10^{-2}$
2	$\frac{1}{4}\sqrt{\frac{5}{\pi}}\left(3z^2 - 1\right)$	$-1.86 \cdot 10^{-3}$	$-2.21 \cdot 10^{-3}$	$-2.44 \cdot 10^{-3}$	$-2.38 \cdot 10^{-3}$	$-2.27 \cdot 10^{-3}$	$-2.09 \cdot 10^{-3}$	$-1.88 \cdot 10^{-3}$
	$\frac{1}{4}\sqrt{\frac{15}{\pi}}\left(x^2 - y^2\right)$	$3.16 \cdot 10^{-4}$	$1.87 \cdot 10^{-4}$	$1.02 \cdot 10^{-4}$	$3.75 \cdot 10^{-5}$	$-2.13 \cdot 10^{-5}$	$-6.78 \cdot 10^{-5}$	$-1.00 \cdot 10^{-4}$
3	$\frac{1}{4}\sqrt{\frac{7}{\pi}}\left(5z^3 - 3z\right)$	$3.03 \cdot 10^{-4}$	$2.25 \cdot 10^{-4}$	$1.20 \cdot 10^{-4}$	$5.22 \cdot 10^{-5}$	$-2.03 \cdot 10^{-5}$	$-1.05 \cdot 10^{-4}$	$-1.96 \cdot 10^{-4}$
	$\frac{1}{4}\sqrt{\frac{105}{\pi}}\left(x^2 - y^2\right)z$	$-1.46 \cdot 10^{-5}$	$-6.82 \cdot 10^{-6}$	$3.17 \cdot 10^{-7}$	$7.91 \cdot 10^{-6}$	$1.44 \cdot 10^{-5}$	$1.96 \cdot 10^{-5}$	$2.16 \cdot 10^{-5}$
4	$\frac{3}{16}\sqrt{\frac{1}{\pi}}\left(35z^4 - 30z^2 + 3\right)$	$-4.60 \cdot 10^{-5}$	$1.26 \cdot 10^{-4}$	$3.38 \cdot 10^{-4}$	$3.63 \cdot 10^{-4}$	$3.71 \cdot 10^{-4}$	$3.57 \cdot 10^{-4}$	$3.17 \cdot 10^{-4}$
	$\frac{3}{8}\sqrt{\frac{5}{\pi}}\left(x^2 - y^2\right)\left(7z^2 - 1\right)$	$2.45 \cdot 10^{-6}$	$9.21 \cdot 10^{-6}$	$1.36 \cdot 10^{-5}$	$7.96 \cdot 10^{-6}$	$3.76 \cdot 10^{-6}$	$1.06 \cdot 10^{-7}$	$-3.83 \cdot 10^{-6}$
	$\frac{3}{16}\sqrt{\frac{35}{\pi}}\left(x^4 - 6x^2y^2 + y^4\right)$	$-5.05 \cdot 10^{-7}$	$-3.87 \cdot 10^{-7}$	$-1.36 \cdot 10^{-6}$	$-2.98 \cdot 10^{-6}$	$-6.45 \cdot 10^{-6}$	$-1.38 \cdot 10^{-5}$	$-2.54 \cdot 10^{-5}$

Mollweide-projection

How to plot an $E(\vartheta, \varphi)$ function?



Mollweide-projection

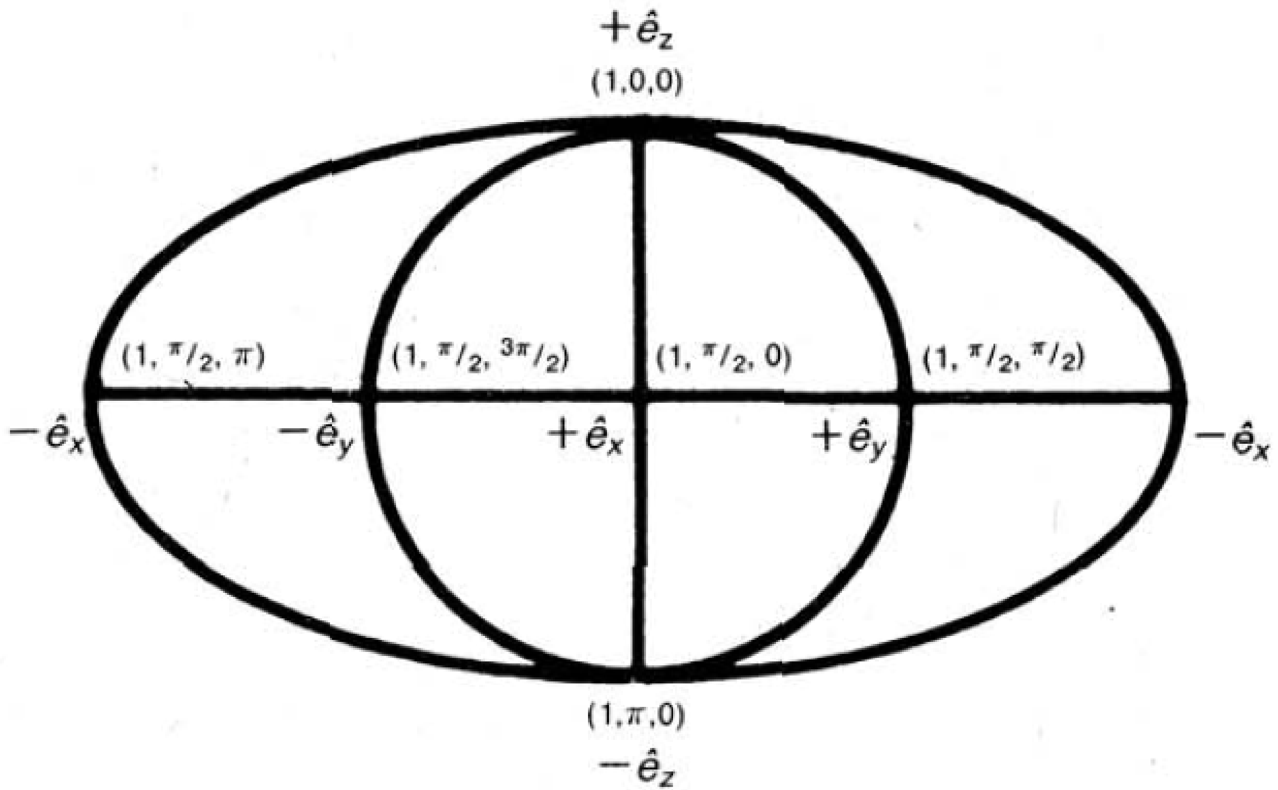


Figure 1. Mollweide's elliptical projection of the unit sphere based on the normal right-handed Cartesian coordinate system viewed towards the coordinate origin from along the $+x$ axis.

$$x = 2\sqrt{2}\,\frac{\varphi}{\pi}\cos(\xi)$$

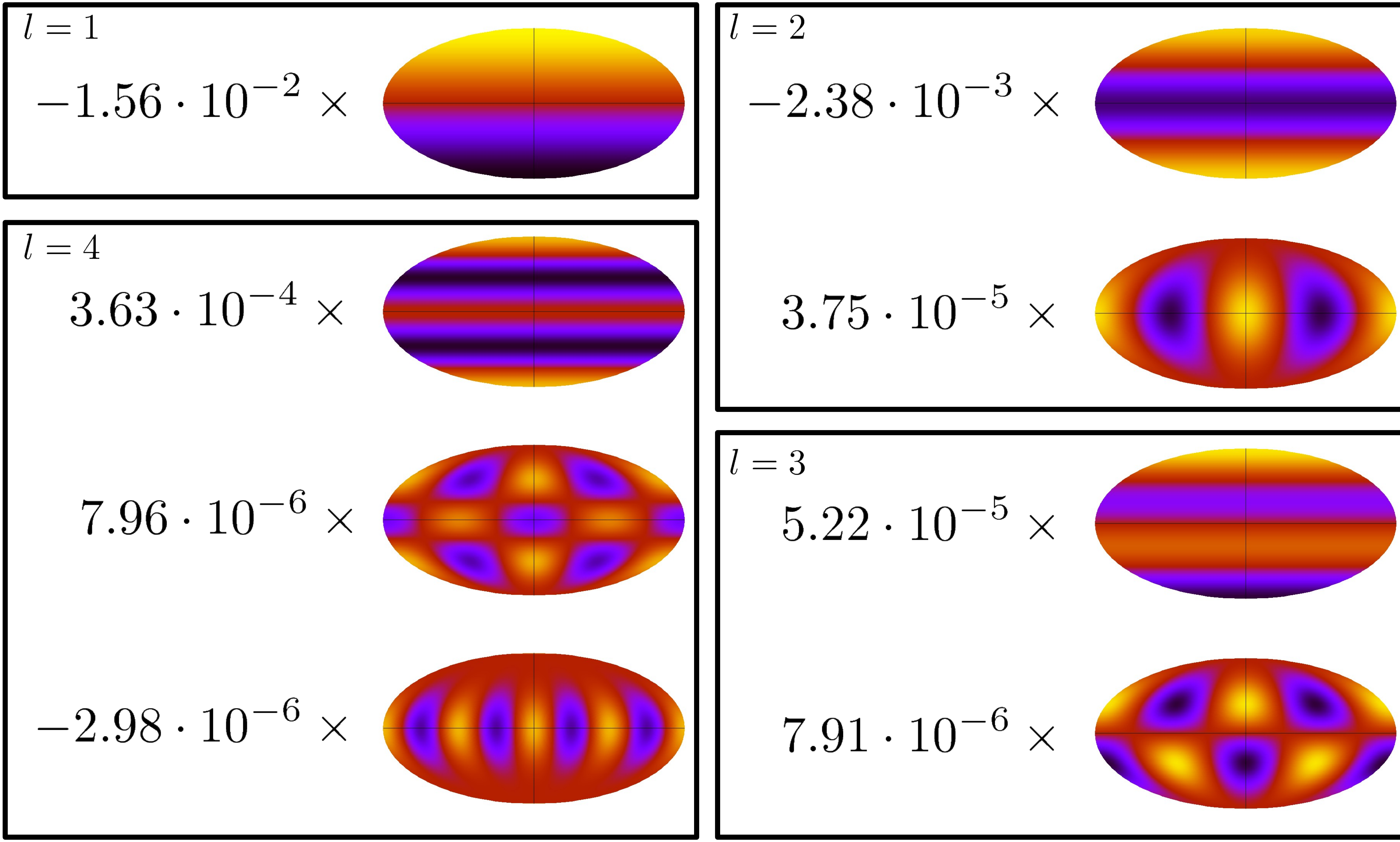
$$y = \sqrt{2}\sin(\xi)$$

$$2\xi + \sin(2\xi) = \pi\cos(\vartheta)$$

C. M. Quinn *et al.*, J. Chem. Edu., **61,** 569, (1984)

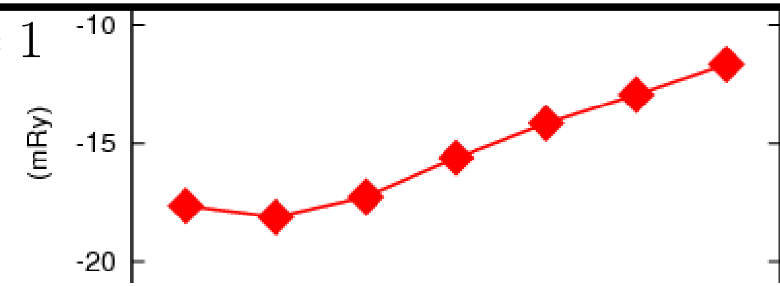
http://en.wikipedia.org/wiki/Mollweide_projection

Decomposition of the energy function [Ryd]

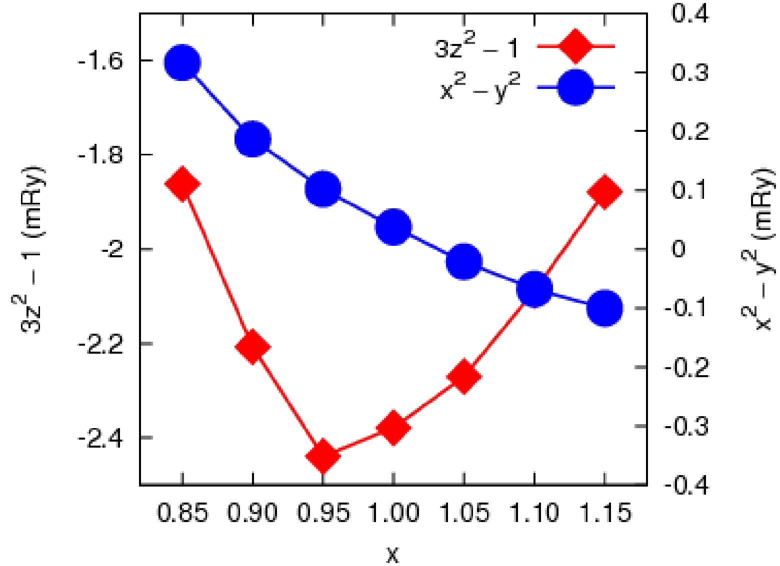


Decomposition of the energy function II.

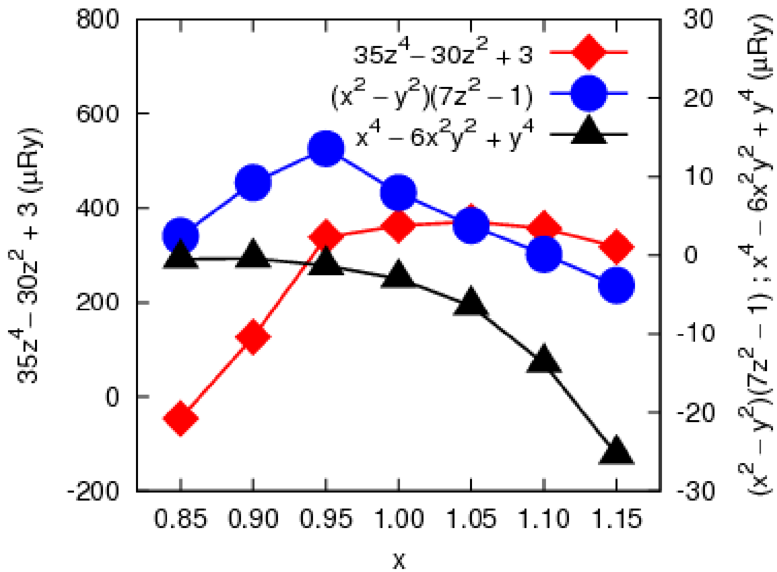
$l = 1$



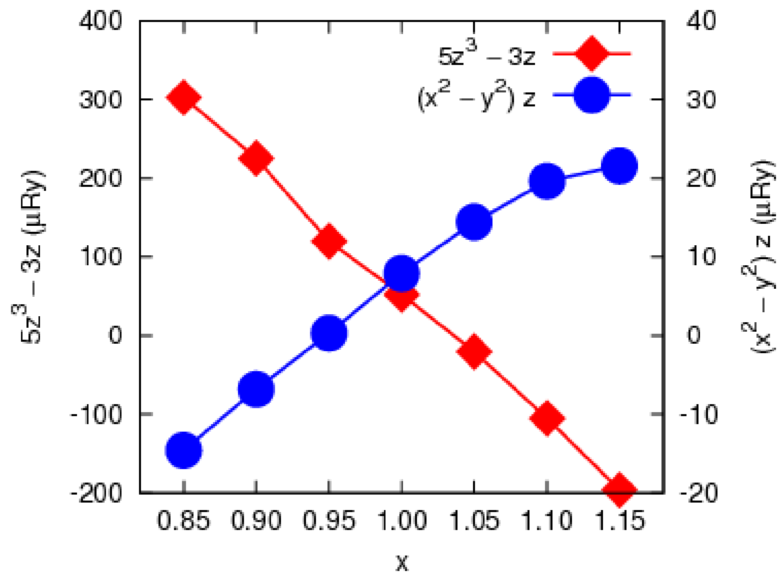
$l = 2$



$l = 4$



$l = 3$

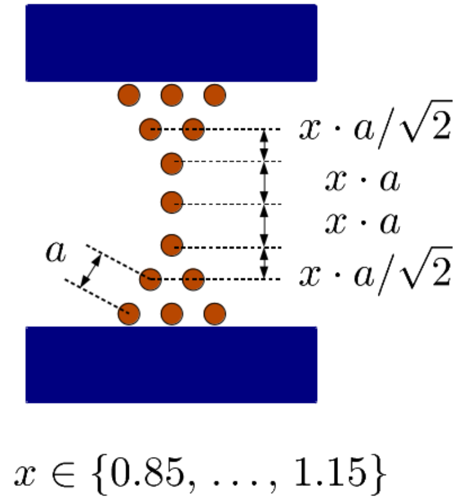


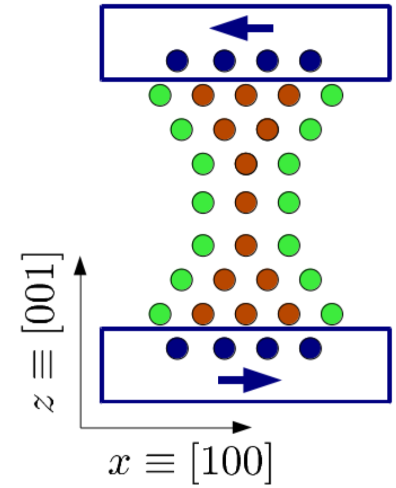
Summary

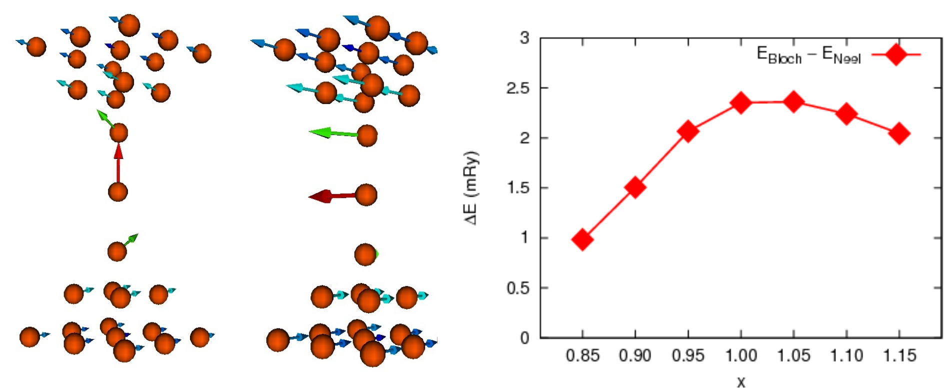
♣ A model of a cobalt nanocontact was constructed and investigated.

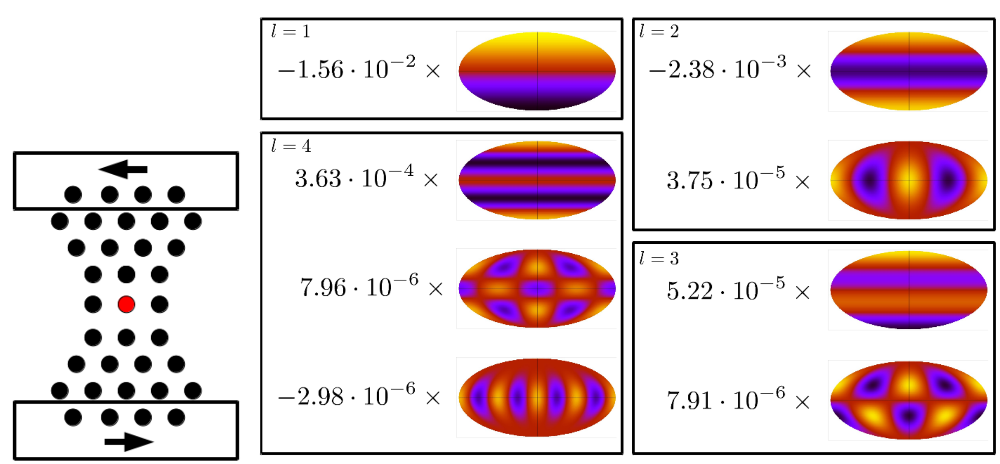
♣ The ground state was searched with multiscale approach: MC simulated annealing + NR optimization of the band energy.

♣ The Heisenberg model is not sufficient to map the magnetic energy landscape.





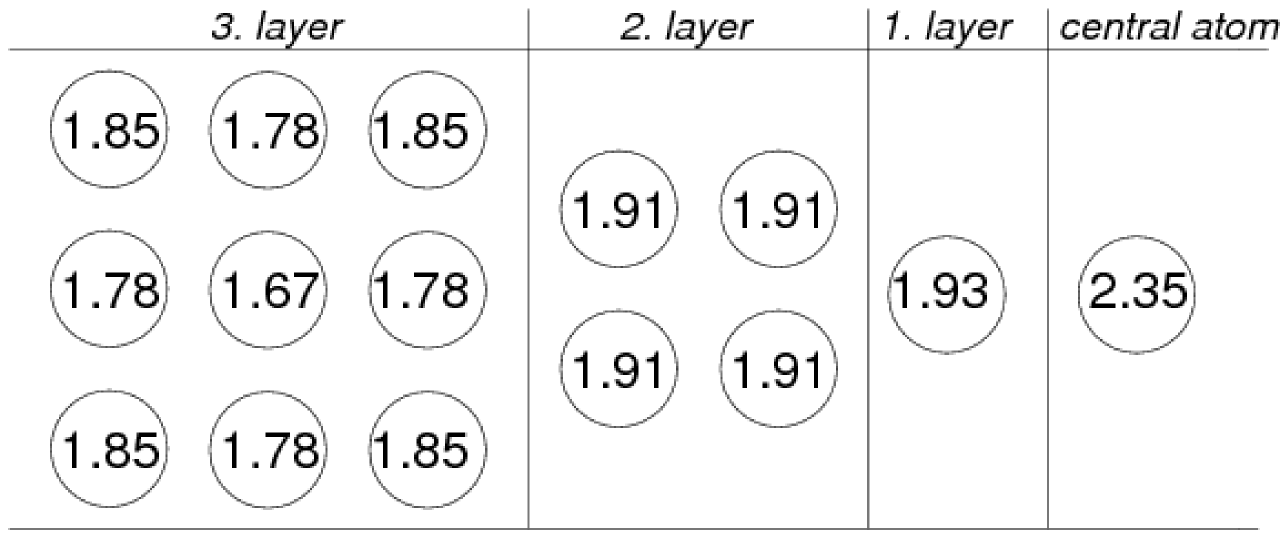


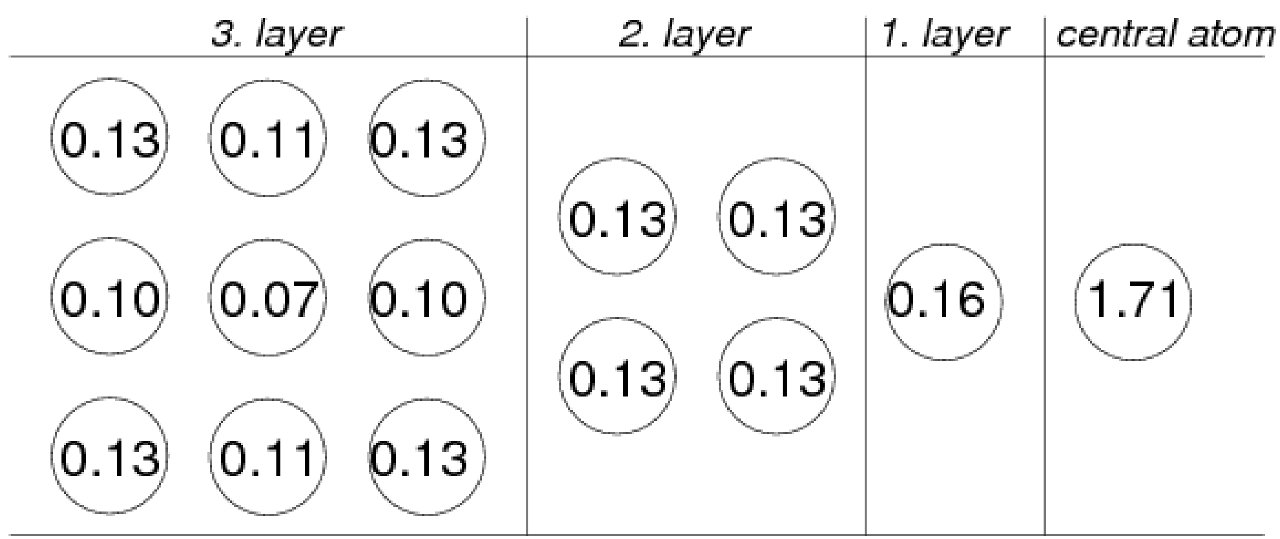


Thank you for your attention

László Balogh, Krisztián Palotás, Bence Lazarovits,
László Udvardi, László Szunyogh

Spin- and orbital moments on the atomic sites. (Néel str., $x = 1.00$)





Spin- and orbital moments on the central atom. (Néel str.)