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To cite this version:

Eszter Simon, Bence Lazarovits, László Szunyogh, Balazs Ujfalussy. Ab initio investigation of RKKY interactions on metallic surfaces. Philosophical Magazine, 2008, 88 (18-20), pp.2667-2672. 10.1080/14786430802322206 . hal-00513935

HAL Id: hal-00513935

https://hal.science/hal-00513935v1

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Ab initio investigation of RKKY interactions on metallic surfaces

Journal:	*Philosophical Magazine & Philosophical Magazine Letters*
Manuscript ID:	TPHM-08-May-0179
Journal Selection:	Philosophical Magazine
Date Submitted by the Author:	21-May-2008
Complete List of Authors:	Simon, Eszter; Research Institute for Solid State Physics and Optics, Theoretical Physics Lazarovits, Bence; Research Institute for Solid State Physics and Optics, Theoretical Physics Szunyogh, László; Budapest University of Technology and Economics, Theoretical Physics Ujfalussy, Balazs; Research Institute for Solid State Physics and Optics, Theoretical Physics
Keywords:	first-principles calculations, magnetism, nanotechnology
Keywords (user supplied):	magnetic interactions
Note: The following files were submitted by the author for peer review, but cannot be converted to PDF. You must view these files (e.g. movies) online.	
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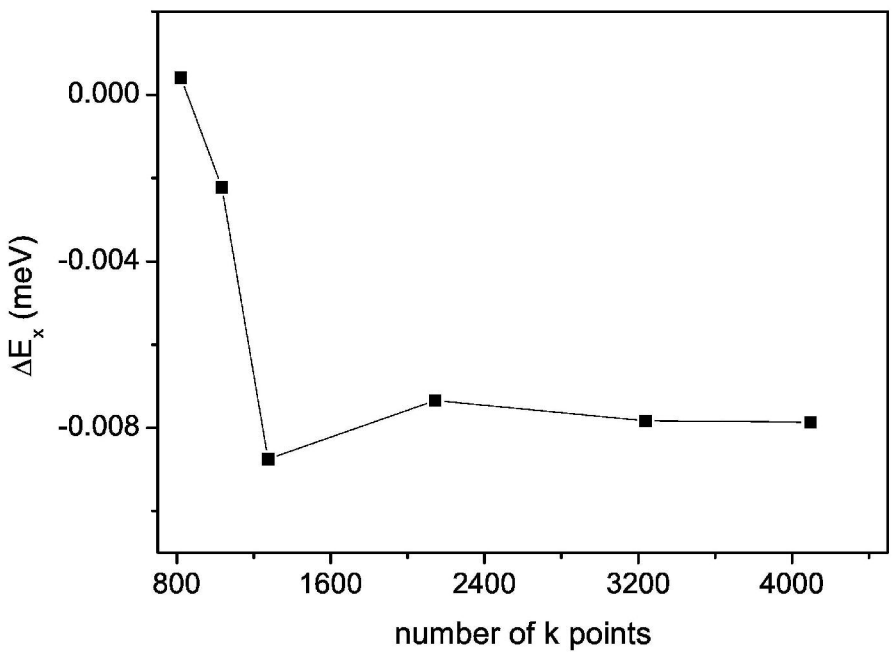

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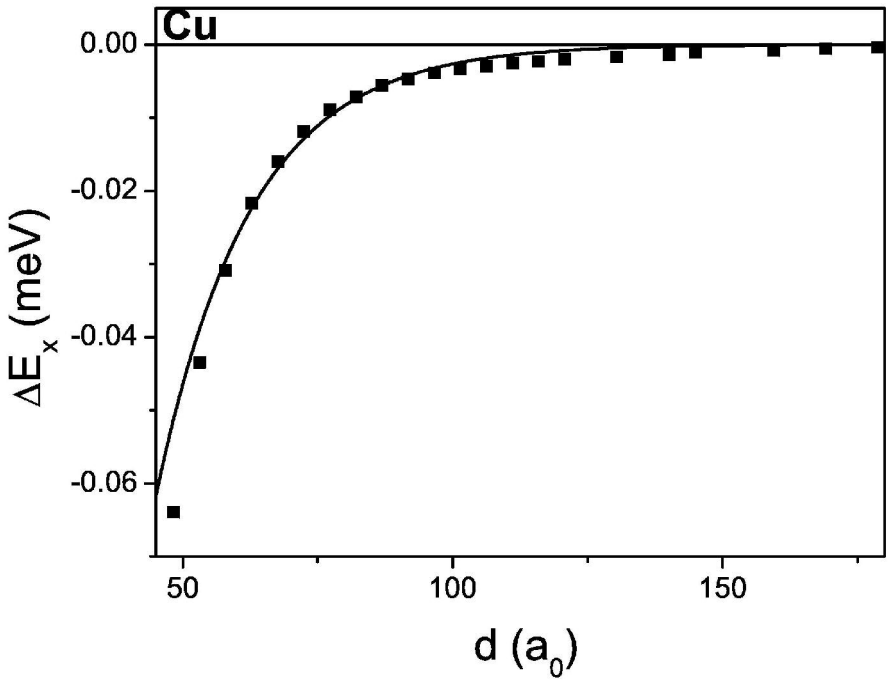

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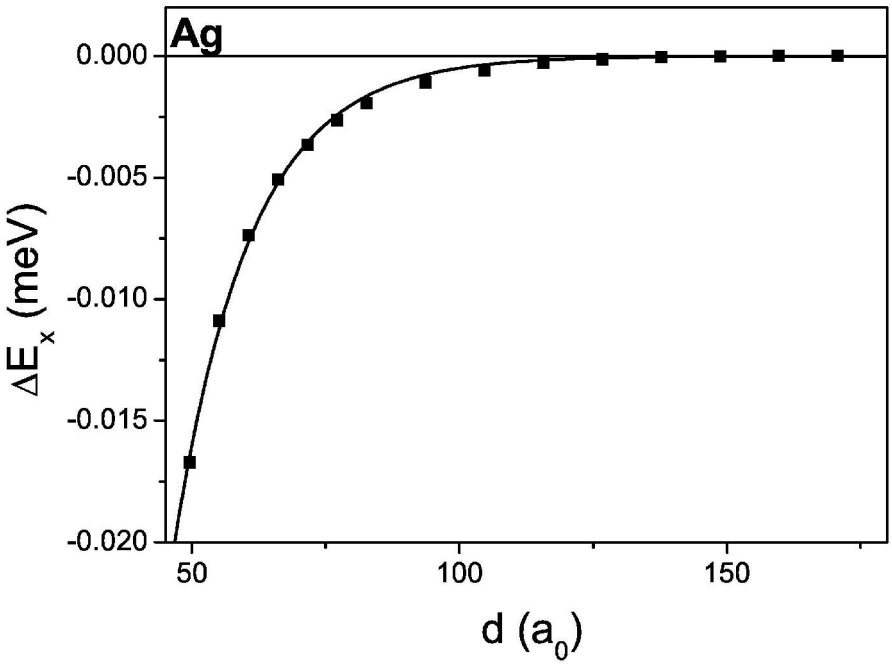

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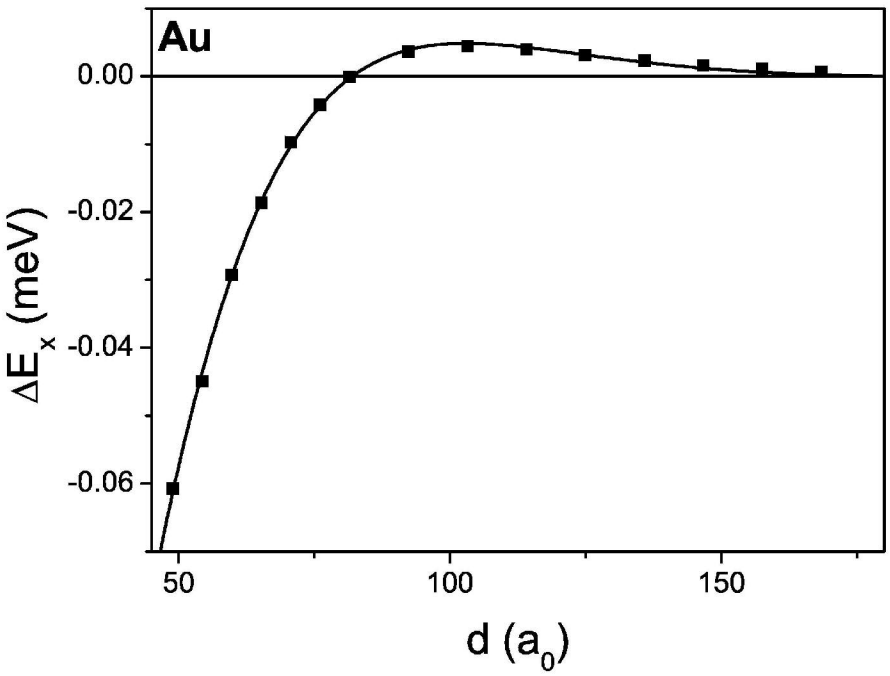

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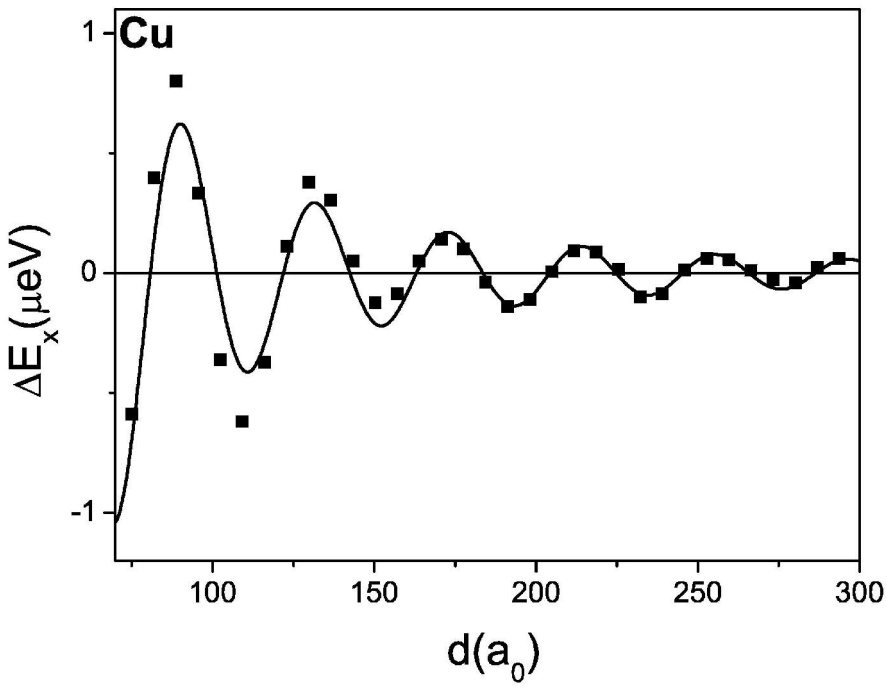

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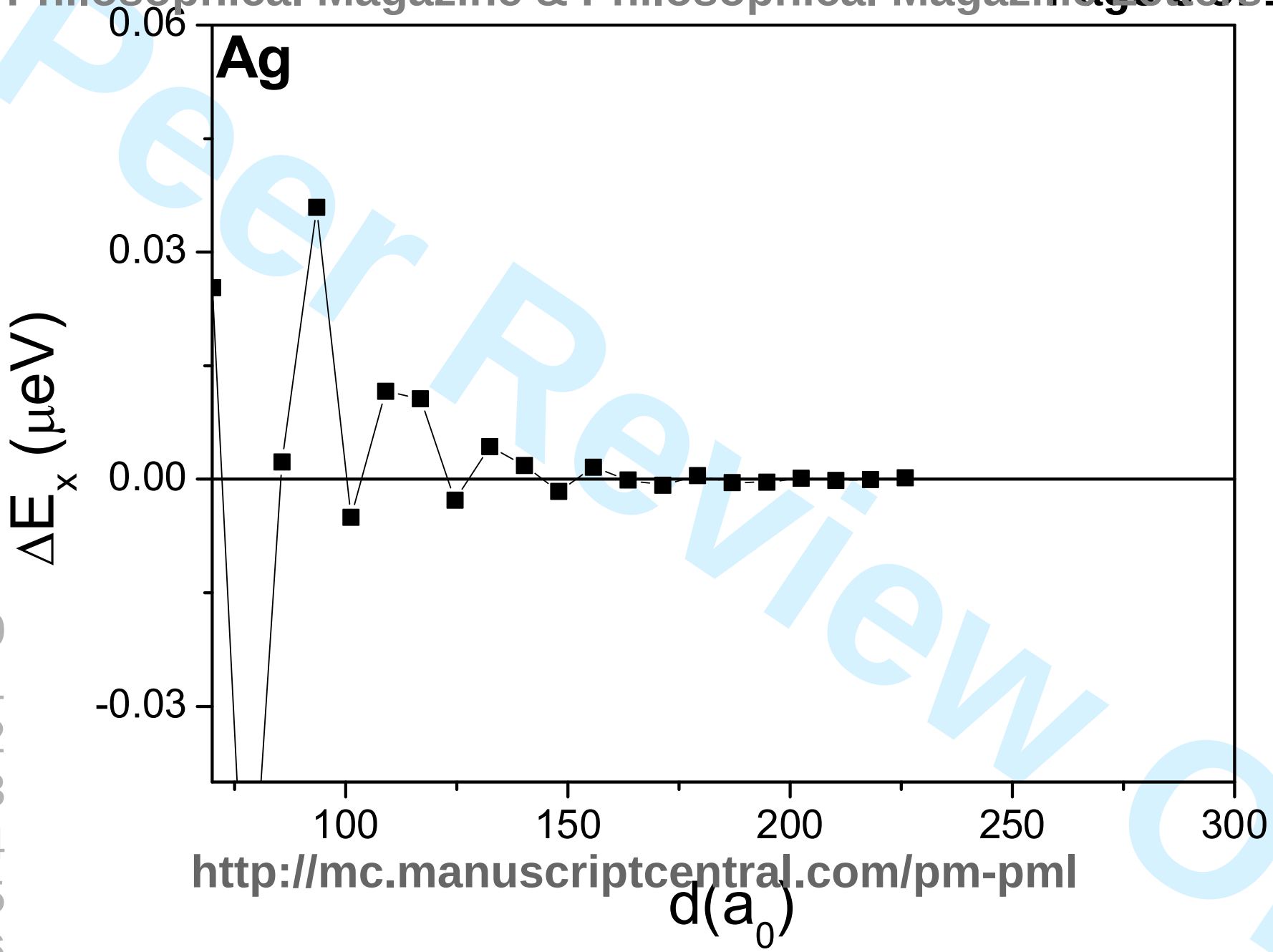

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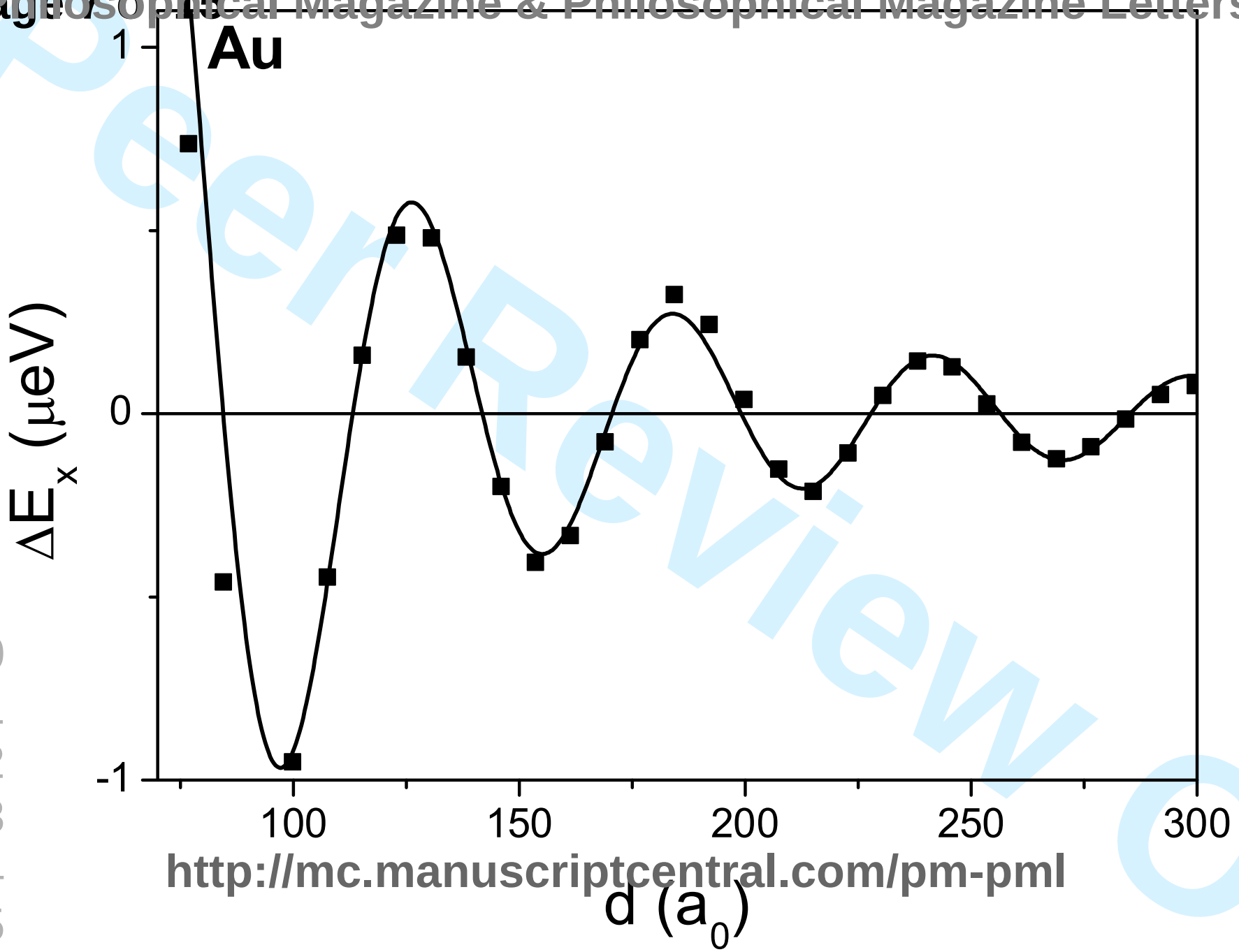

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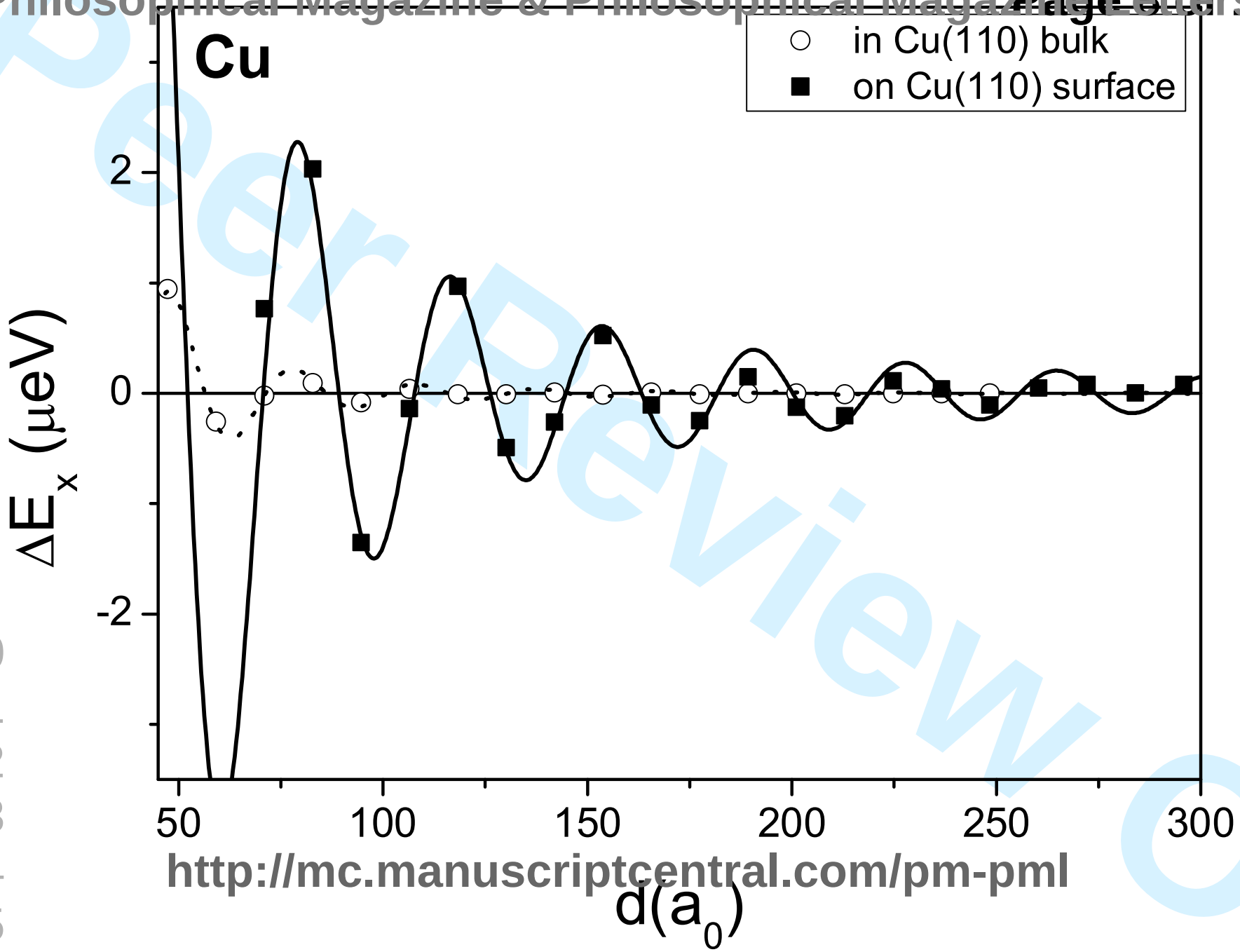

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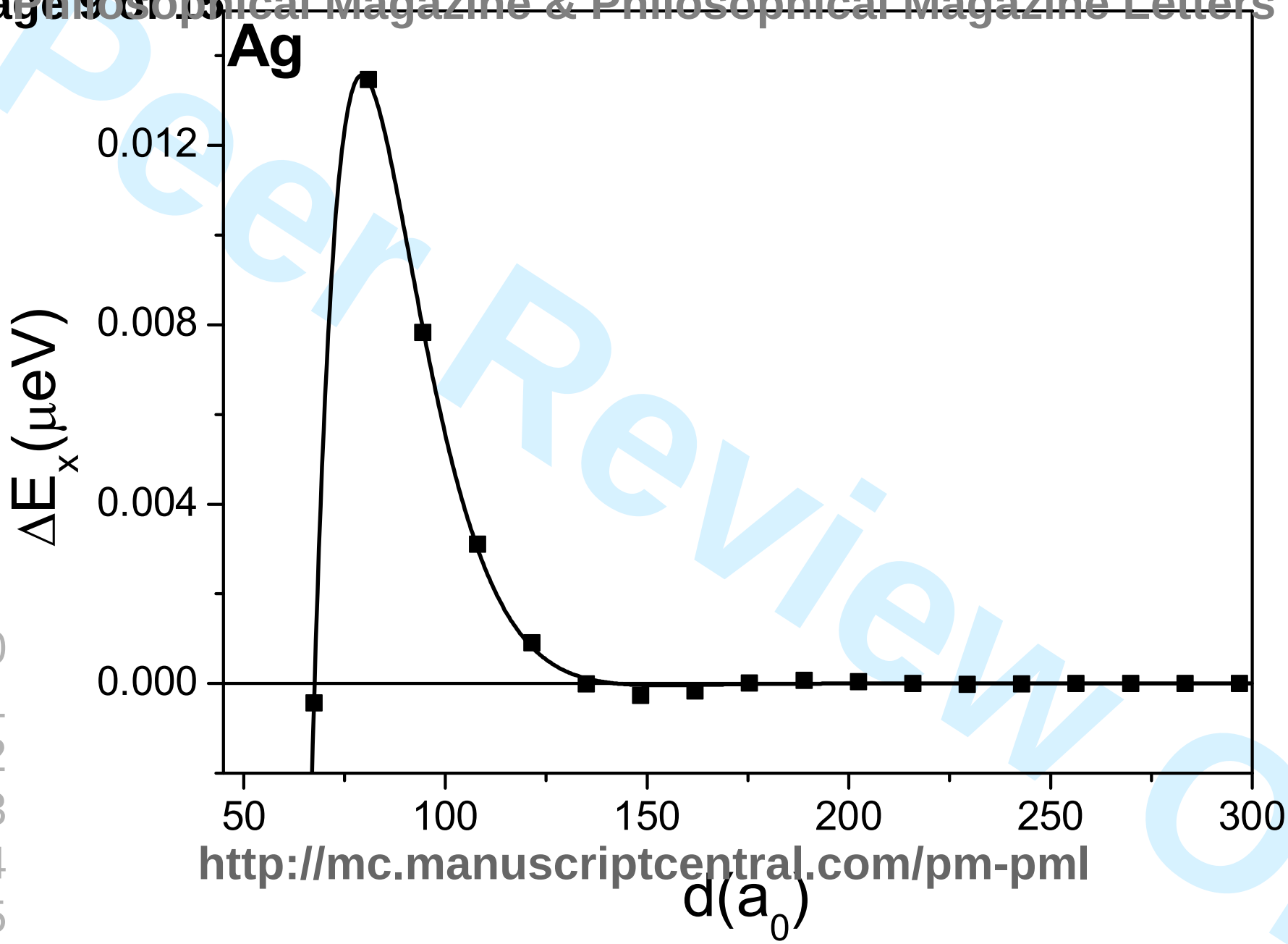

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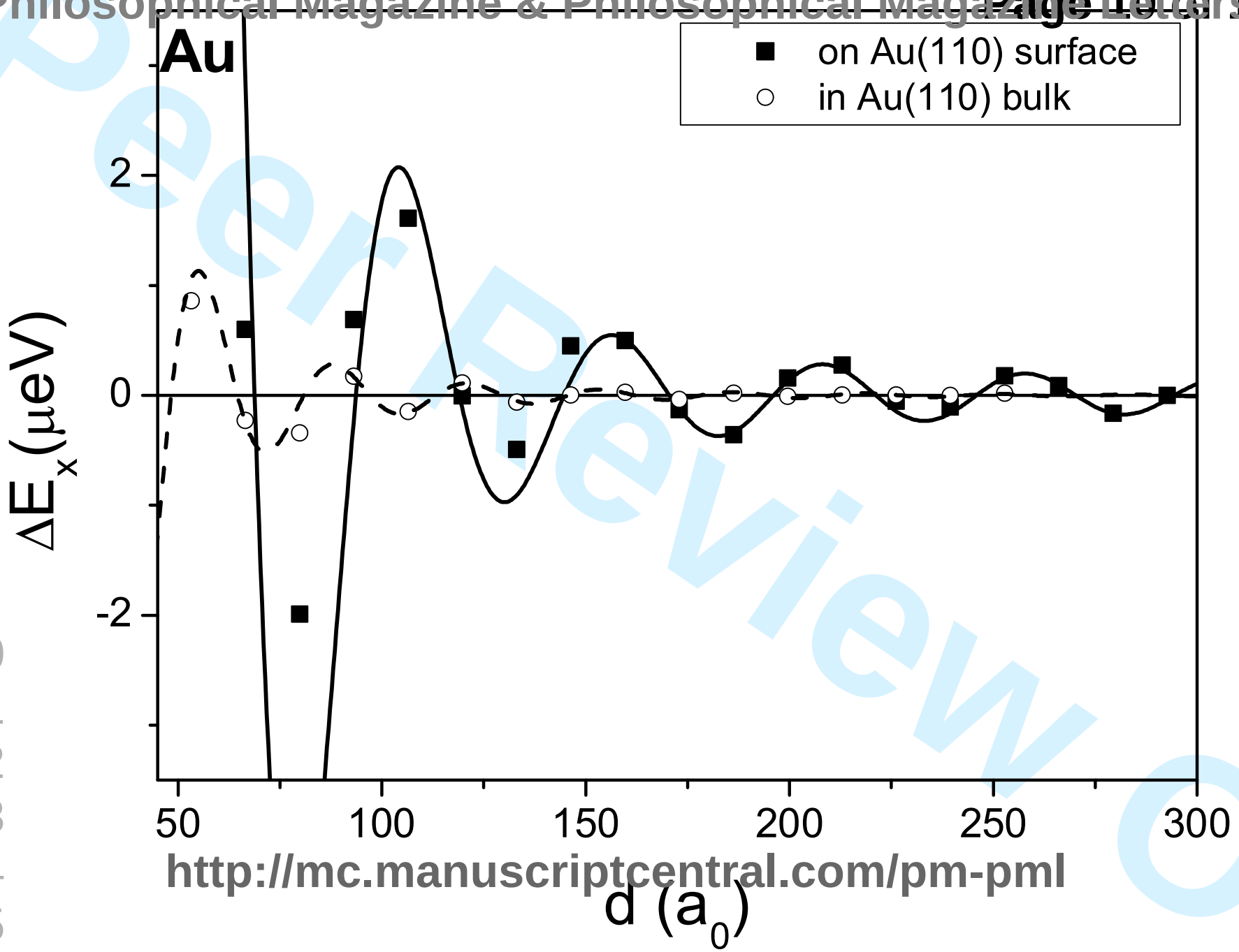

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Philosophical Magazine
Vol. 00, No. 00, 00 Month 200x, 1–5

RESEARCH ARTICLE

Ab initio investigation of RKKY interactions on metallic surfaces

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(*Received 00 Month 200x; final version received 00 Month 200x*)

We present ab initio results concerning the RKKY interaction between two Co atoms placed on Cu, Au and Ag surfaces putting the main emphases on its dependence on the supporting material. Calculations based on the screened Korringa-Kohn-Rostoker (KKR) framework combined with the embedding technique are presented for FCC (100) and (110) surfaces. A test for the convergence properties with respect to the Brillouin zone integration is also shown in a selected case.

Keywords: magnetism, nanotechnology, first-principles calculations

1. Introduction

Magnetic nanostructures are in the forefront of current spin-device research. The interaction between such nanostructure, or atoms forming a nanostructure therefore is also of primary importance. In a non-magnetic bulk host material there is a long range interaction between two magnetic impurities known as the RKKY interaction, $E_{RKKY} = J(x)\mathbf{S}_1\mathbf{S}_2$, ($\mathbf{S}_1$ and $\mathbf{S}_2$ are the impurity spins) after Ruderman, Kittel, Kasuya, and Yoshida [1],[2]. This interaction mediated by the conduction electrons of the host, and can be written in the asymptotic limit as

$$J(\mathbf{x}) \approx \frac{cos(2\mathbf{k}_F\mathbf{x})}{x^3} \tag{1}$$

where the $\mathbf{x}$ is the vector connecting the two impurities, and $\mathbf{k}_F$ is the extremal spanning vector of the appropriate cut of Fermi surface of the host. The interactions between two magnetic multilayers appears to have a similar form, also mediated by the conduction electrons of the - bulk like - spacer material, however the exponent of the decay is different [7]:

$$J(\mathbf{x}) \approx \frac{cos(2\mathbf{k}_F\mathbf{x})}{x^2} \tag{2}$$

.

The question obviously arises wether there existed a similar interaction between surface impurities, and whether their behavior was similar? Such a research task

ISSN: 1478-6435 print/ISSN 1478-6443 online
© 200x Taylor & Francis
DOI: 10.1080/1478643YYxxxxxxxx
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nowadays is not even academic. Recent experiments by Wiesendanger [3] showed, it is possible to place two impurities on surfaces, and directly observe their interaction energies experimentally.

Although some attempts have been made before to calculate these interactions, they were usually linked to the (111) surface state [4], [5]. In this paper we present calculations for the (100) and (110) surfaces.

2. Theory

A self-consistent, relativistic calculation has been performed for a single Co atom on the surface using the embedded-cluster technique [6] within multiple scattering theory (MST) which enables the treatment of a finite cluster of impurities embedded into a two-dimensional translationally invariant semi-infinite host. Generally speaking, within MST the electronic structure of a cluster of embedded atoms is described by the so-called scattering path operator (SPO) matrix given by the following Dyson equation

$$\tau_C(\epsilon) = \tau_h(\epsilon)[1 - (t_h^{-1}(\epsilon) - t_C^{-1}(\epsilon))\tau_h(\epsilon)]^{-1} \tag{3}$$

where $\tau_C(\epsilon)$ comprises the SPO for all sites of a given finite cluster C embedded in a host system, $t_h(\epsilon)$ and $\tau_h(\epsilon)$ denote the single-site scattering matrix and the SPO of the unperturbed host sites in cluster C, respectively, while $t_C(\epsilon)$ stands for the single-site scattering matrix of the impurity atoms. Once $\tau_C(\epsilon)$ is known all corresponding local quantities, i.e., charge and magnetization densities, spin and orbital moments, as well as the total energy can be calculated. In all cases the atomic sphere approximation (ASA) was applied.

During the selfconsistent calculations the "cluster of embedded atoms" consisted of a single Co atom. Here we were also using the local density functionals of Ceperley-Alder (in the parameterisation due to Perdew and Zunger) [8] and solving the Poisson equation was solved as described in [9]. During these (single impurity) calculations the direction of the magnetization of the Co atom was kept normal to the surface (z axis), and all relaxation of the impurity atom was neglected. Once a self-consistent potential for a single Co atom has been obtained, we used the magnetic force theorem to calculate the interaction energy:

$$\Delta E = E_{band}(\uparrow,\uparrow) - E_{band}(\uparrow,\downarrow) \tag{4}$$

where E_{band} denotes the band energy contribution to the total energy. The band energies were calculated by embedding two impurity atoms with these potentials twice: once with a ferromagnetic, once with an anti-ferromagnetic spin-alignment.

To calculate the host τ_h tau matrices we used 4 000 k-points in the irreducible wedge of the Brillouin zone. Energy integrations were performed using 16 energy points along a semicircular logarithmic mesh. It is well known, that in the case of inter-layer exchange coupling, to calculate the interactions in the asymptotic regime, an extreme care had to be taken to make the appropriate Brillouin zone integrations converge. It is expected, that if the mechanism of the interactions is indeed similar, a similar convergence problem will occur in calculating the interactions between surface impurities. Therefore we tested the convergence of our calculations up to 4000 k-points in the irreducible wedge of the brillouin zone as shown on Figure 1.

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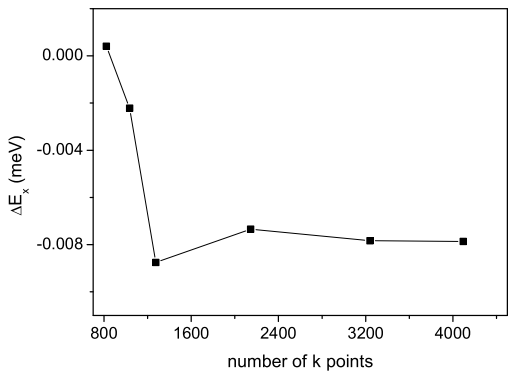

Figure 1. Convergence of the exchange interaction energy between two Co impurities on the FCC Au(100) surface with respect to the number of the k-points in the irreducible wedge of the Brillouin zone. The impurities were placed apart by 20 lattice constants

3. Results for a Co impurity on Cu, Ag and Au surfaces

In Figure 2, the exchange interaction energies for two Co atoms placed on the (100) surface of FCC Cu, Ag and Au are shown as functions of the distance between the adatoms. The two Co atoms were pulled apart along the nearest neighbor direction (x axis) of the 2D square lattice. It should be noted that because of the point group symmetry of the surface, the x and y directions are equivalent in this respect. This symmetry argument has been verified by the actual calculations. It can be seen that the interaction between the two impurities decay exponentially for all hosts. The interaction still present must come from direct overlap of the impurity orbitals, which, however decays exponentially. Therefore, we may conclude that on the contrary to the corresponding bulk systems, there is no long-ranage oscillatory RKKY type magnetic interaction between the magnetic atoms on the (investigated) (100) surfaces.

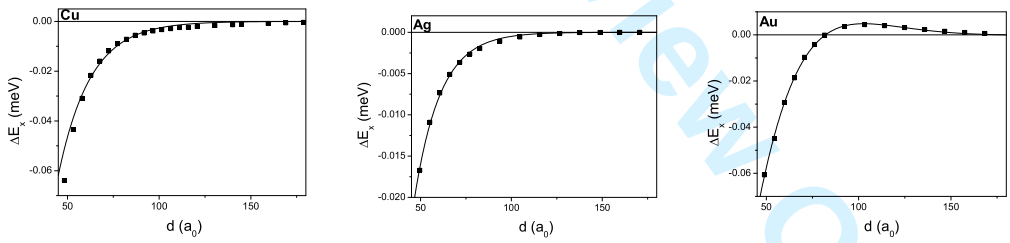

Figure 2. Exchange interaction between two surface impurities as a function of distance along the x-axis on the surfaces of Cu(100), Ag(100), Au(100). The dots show the calculated energies and the full lines are the fitted curves with exponential decay.

The situation is quite different on the (110) surface. First of all, the generating vectors of the two-dimensional lattice are $\mathbf{a}_1 = (a, 0)$ and $\mathbf{a}_2 = (0, 1/\sqrt{2}a)$ where a is the 3-dimensional lattice constant. We performed calculations for two different surface directions: one along the x axis, and one along the $2\mathbf{a}_1 + \mathbf{a}_2$ direction which is equivalent to the (111) direction in the bulk. The calculated interaction energies are shown in Fig. 3 for the case where the two impurities were pulled apart along the x direction. First, it should be noted that on Ag(110) the interaction shows an entirely different behavior than the other two cases: after a few oscillations it becomes negligibly small. This behavior can probably be linked to the positions of the sharp d-type resonances of the Co ad-atoms relative to the bands of the Ag

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surface.

On Cu and Au, it can be seen that the interactions do show a marked oscillatory behavior. The oscillations can be fitted with a function, which has a decay slightly different from the bulk RKKY form: $f(x) \approx \frac{1}{x^2} cos(kx)$.

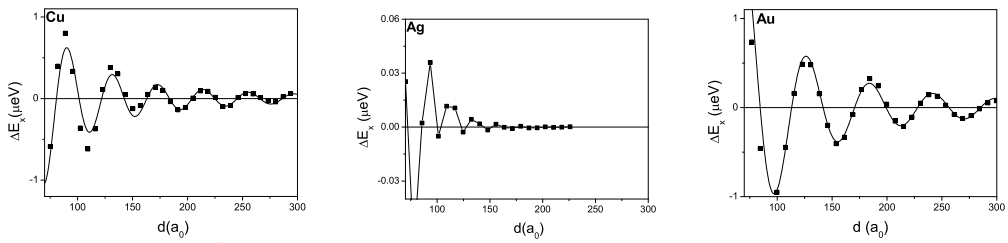

Figure 3. Exchange interaction energy between two surface impurities as a function of distance along the x-axis on the surface of Cu(110), Ag(110), Au(110)

Second, on figure 4 we plotted the interaction energies when the impurities were pulled apart along the bulk (111) direction. We again find that in case of Ag, there is a very fast decay of the interaction, even more characteristic as in the case of the (110) surface. On the other two substrates one can again observe an oscillatory RKKY type interaction which can be fitted with a similar kind of function as previously. This direction offers an easy comparison with bulk RKKY oscillations, where the wave-length of the oscillations can be easily compared to the diameter of the "neck" in the corresponding bulk Fermi surfaces. In Figure 4 we also plotted the RKKY interactions in bulk Cu and Au (hollow symbols, dashed line). One can immediately see, that the amplitude of the interaction is greatly magnified on the surface. Additionally, the oscillatory interaction decays like $\frac{1}{x^2}$ - again the interactions decays slower on the surface then in the bulk. It should be mentioned, that in our bulk calculations the diameter of the "neck" of the bulk Cu and Au Fermi surfaces are correctly reproduced by the frequency of the curve fitted to the oscillatory interaction.

One can also see, that the frequencies of the oscillatory interactions are similar on the surface and in the bulk, while the phase and amplitude differs considerably. This indicates a similar mechanism, the interaction being mediated by the conduction electrons penetrating deep into the host material.

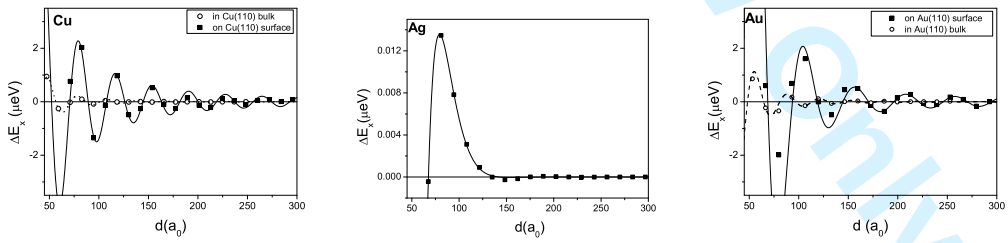

Figure 4. Exchange interaction between two surface impurities as a function of distance along the bulk (111) direction on the surface of Cu(110), Ag(110), Au(110)

4. Conclusions

While analytical or semi-analytical calculations for the RKKY interaction between two impurities in the bulk, or the oscillatory exchange coupling is rather easy

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to obtain, and is numerous in the literature, for the general case of the surface impurities it is not so. The reason to this lies in the fact that an (analytical) derivation of a Green's function of a semi-infinite surface, or other methods to model the semi-infinite substrate is hard to obtain. Therefore, ab-initio calculations provide an excellent way to discover the principles governing the interactions, and helping the experimental efforts.

In this paper we presented first-principles based calculations for the exchange interaction energies between two magnetic impurities based on the magnetic force theorem. We found that in contrary to the in-bulk interactions, on the (100) surface there is no long-range oscillatory interaction between two impurities on either Cu, Ag or Au. However, on the (110) surface of Cu and Au, the oscillatory interaction considerably strengthens compared to the in-bulk ones, and decays according to a $\frac{1}{x^2}$ power law.

Acknowlegemets

Financial support to this work was provided by the Hungarian National Science Foundation under Contract Number OTKA K-68312 and F-68726.

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