Magnetism of Fe Surface

First-principles calculations reveal that the magnetic moments of atoms on an Fe(001) surface are 30% larger than in the bulk. This enhancement decays within about three layers towards the bulk, which demonstrates the highly localized character of enhanced surface magnetism in transition metals such as iron.

Keywords: Magnetism, surfaces, iron, first-principles, computations

Background

With the development of accurate surface science techniques in the late 1960's initial experimental data suggested "magnetically dead" layers on transition metal surfaces. By the late 1970's and early 1980's first-principles methods combined with the power of supercomputers of that time allowed for the first time accurate calculations of magnetic properties of surfaces. These calculations indicated enhanced magnetic moments at the Fe surfaces [1,2] in contradiction to experiments. There was no reason to doubt the reliability of these calculations. The discrepancy was later traced to surface contamination and further experiments reconciled the theoretical and experimental data as discussed in Ref. [3].

Computed Results

The magnetic moment of iron atoms on a (001) surface is computed to be 2.92 μ_B with an oscillatory decay towards the bulk as given in Fig. 1. The spin density of the surface atoms has an oval shape while the Fe atoms in the interior of the film exhibit a more square-like form (see Fig. 1). The present calculations give a value of 2.24 μ_B for bulk Fe, which is close to the experimental value of 2.12 μ_B .

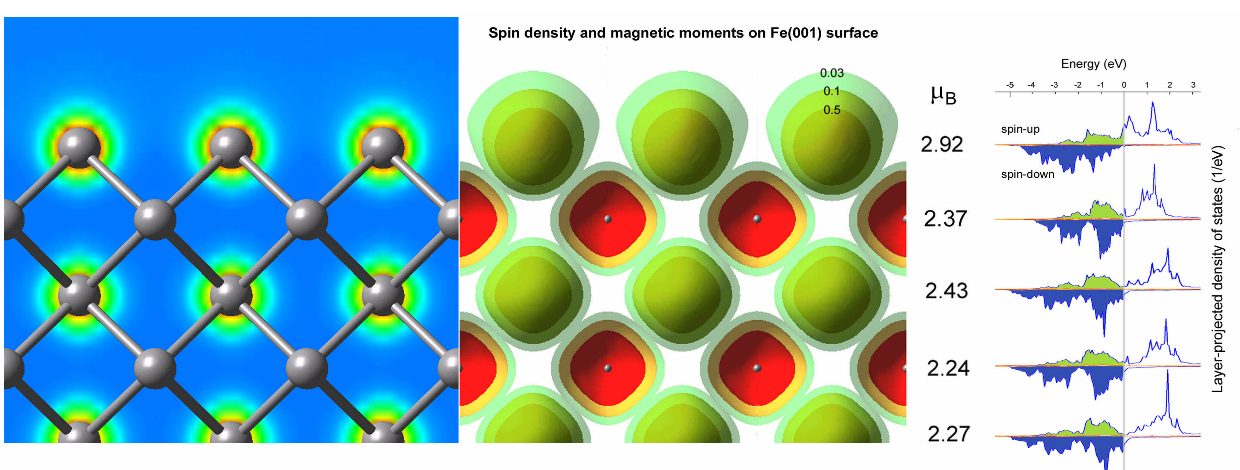

Figure 1. Spin density at an Fe(001) surface in a cut perpendicular to the surface. The left panel shows a contour plot in a (110) plane. The central panel displays the spin density as three-dimensional iso-contours at values of 0.03, 0.1 and 0.5 el/Å^3. The layer-projected electronic densities of states are shown on the right.

Significance

Magnetic properties are of critical importance for our information-based society. Tremendous amounts of data such as business and banking information, email correspondence, contact information, digital images and movies are stored on magnetic disks. Furthermore, permanent magnets are essential for all kind small and large electric motors, which may have significant impact on the performance of future electric cars. Spintronics, *i.e.* the combined use of electronic and magnetic properties is emerging as a new technology in microelectronics. Related to this phenomenon was the discovery of the giant magneto-resistance effect by Peter Grünberg and Albert Fert in 1988, which brought about a breakthrough in gigabyte magnetic disks. For their work these researchers were awarded the Nobel prize in 2007.

First-principles calculations are a reliable source for predicting magnetic properties as demonstrated here for the prototypical case of an Fe(001) surface. Given the performance and continuing evolution of computing power, magnetic properties of increasing complex systems such as nanostructures can be predicted with high confidence, thus guiding the design of novel materials and devices.

MedeA modules used for this application

The present calculations were performed with the MedeA platform using the following integrated modules of the MedeA software environment

- MedeA framework including crystal structure builders, surface builder, and analysis tools for spin densities and electronic densities of states.
- JobServer and TaskServers
- VASP 5.2 and its graphical user interface as integrated in MedeA

References

1. C.S. Wang and A. J. Freeman, Phys. Rev. B **24**, 4364 (1981)
2. S. Ohnishi, A. J. Freeman, and M. Weinert, Phys. Rev. B **28**, 6741 (1983)
3. N. B. Brookes, A. Clarke, P. D. Johnson, and M. Weinert, Phys. Rev. B **41**, 2643 (1990)
4. G. G. Lonzarich, *Electrons at the Fermi Surface*, Ed. M. Springford, Cambridge University Press, Cambridge, p. 225 (1980)

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