Magnetic structure of iron clusters and iron crystal surfaces

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Introduction

- Clusters comprising few tens or hundreds of atoms bridge between atoms and molecules on the one hand and solids on the other hand.

- Clusters contain a large portion of surface atoms.

- Our aim is to learn more about the relation between electronic and magnetic properties of atoms which are close to a cluster surface and of atoms which are close to the planar surface of a crystal.

- Fully relativistic *ab-initio* calculations $\rightarrow$ spin-orbit-coupling induced properties, such as orbital magnetic moments, are treated consistently.

Theoretical methods

- Free 89-atoms spherical-like cluster constructed from the first 7 coordination spheres of bulk bcc Fe, surrounded by 48 empty spheres.
- Half-crystal simulated by a 2D finite slab of 18 planes with Fe atoms and 7 planes with empty spheres on both sides.
- Magnetization parallel to the [001] direction of the parental crystal, i.e., perpendicular to the slab surface.
- Fully-relativistic spin-polarized calculations.
- Cluster: multiple-scattering technique with ASA, as implemented in the SPRKKR code *[H. Ebert, in Electronic structure and physical properties of solids. H. Dreyssé (Ed.), Springer, Berlin, 2000, p. 191]*.
- Surface: tight-binding KKR method *[R. Zeller, P. H. Dederichs, B. Újfalussy, L. Szunyogh, P. Weinberger, Phys. Rev. B* **52***, 8807 (1995)]*.

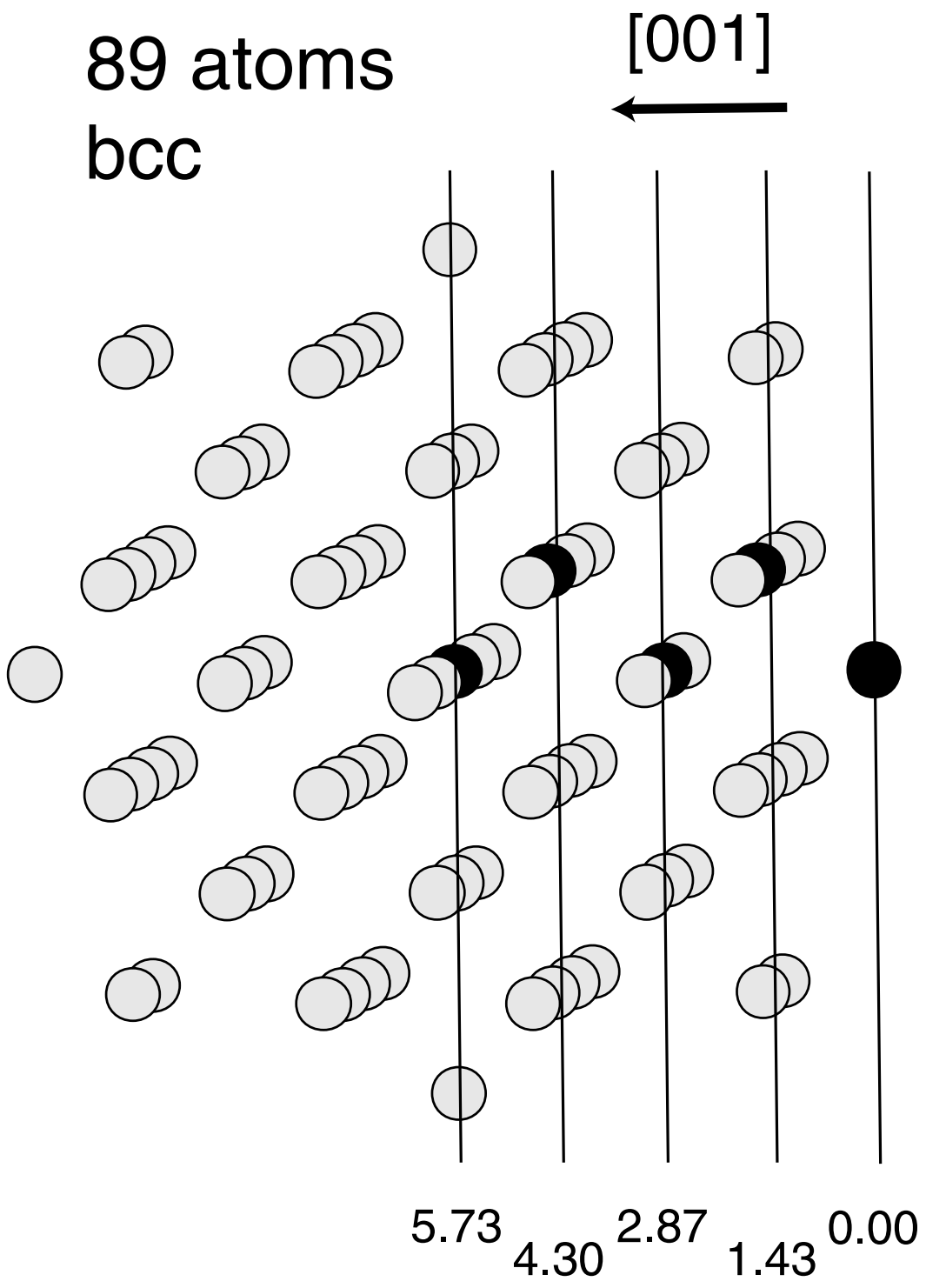


Figure 1: 89-atoms cluster with (001) crystal planes schematically depicted. Numbers below the planes are distances in Å of the respective plane from the "surface plane". Atoms selected as representing each plane are shown in black.

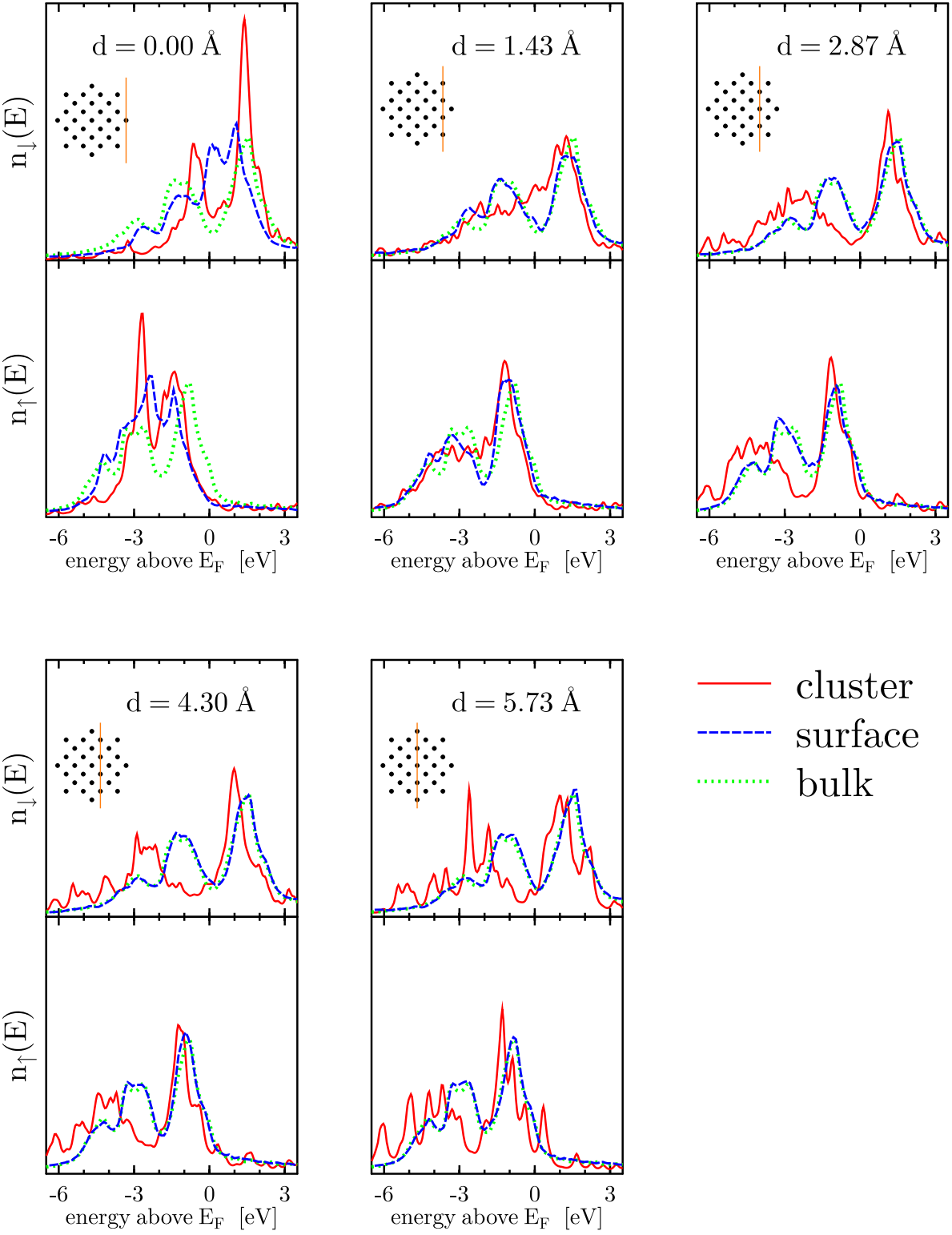
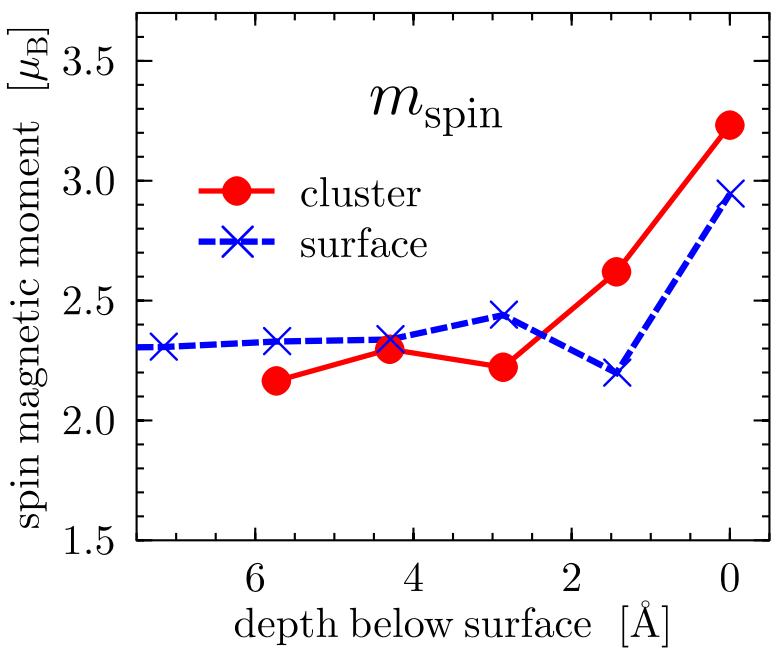


Figure 2: Spin-polarized DOS of atoms in the cluster (red lines) and at and below the (001) crystal surface (blue lines). Green lines show DOS of the bulk Fe-crystal. The distance d from the surface as well as the position of the relevant layer in the 89-atoms cluster are shown in the insets.



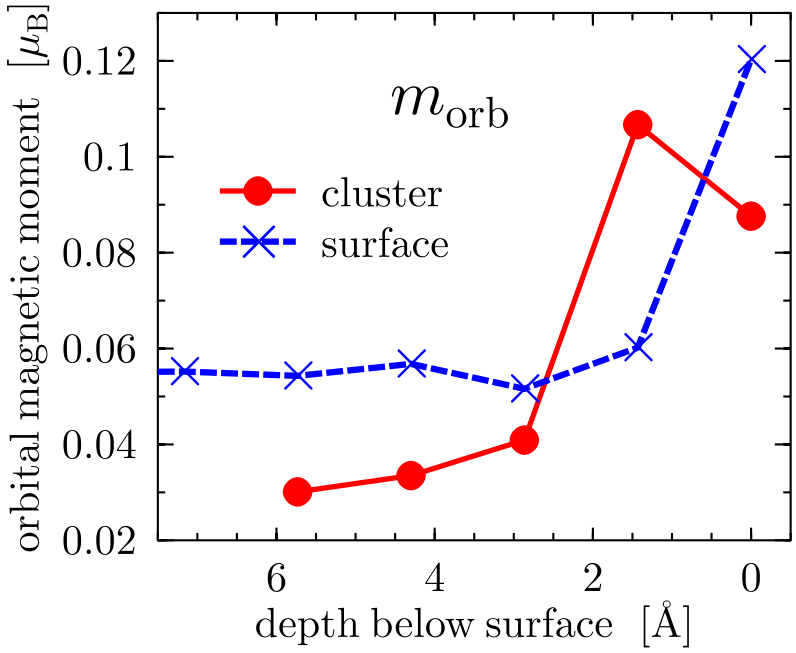


Figure 3: Dependence of the spin magnetic moment m_{spin} and orbital magnetic moment m_{orb} in a 89-atoms cluster (red lines) and in a half-crystal (blue lines) on the distance below the (001) surface.

Conclusions

- The depth-profiles of an 89-atoms iron cluster and of a (001) iron crystal surface exhibit different behaviour both as concerns DOS and the magnetic moments.

- The electronic properties of atoms at a surface of a cluster display more pronounced atomic-like features than atoms at a surface of a crystal.

- The convergence of DOS and of both m_{spin} and m_{orb} towards the bulk values is much faster for a planar (crystal) surface than for a cluster.