Fe adatom along Bi nanolines on H/Si(001): Patterning atomic magnetic chains

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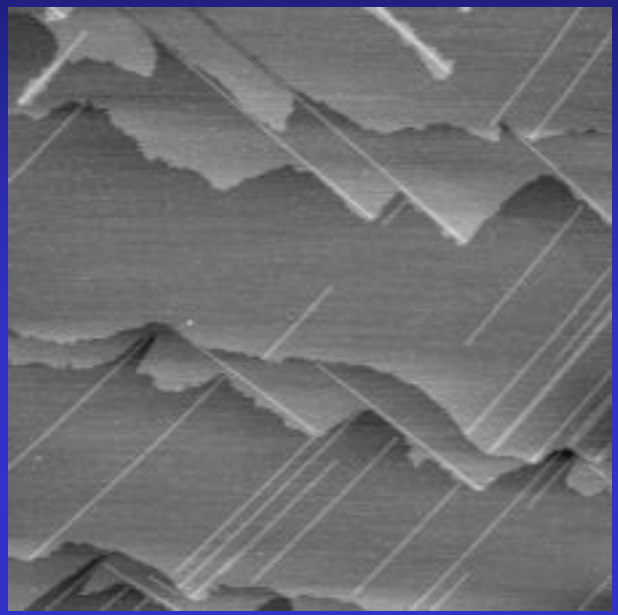
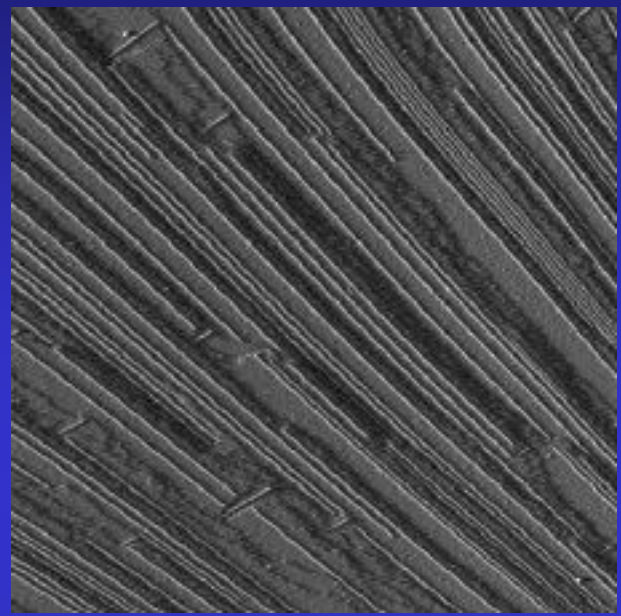
Outline

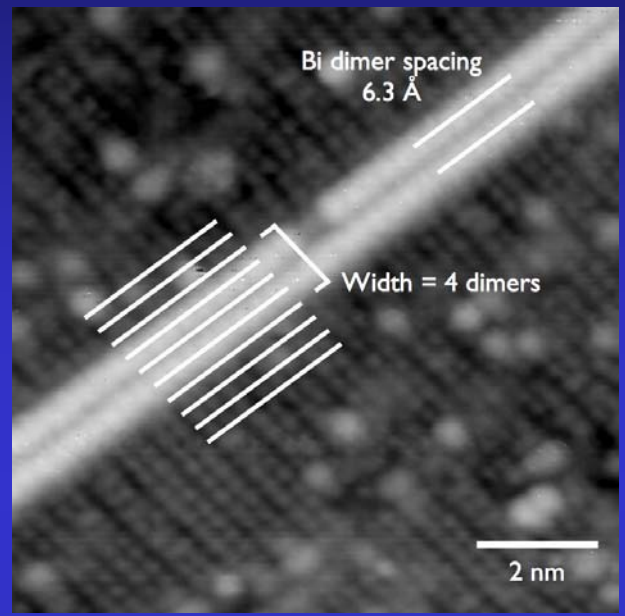
- Self-organized 1D structure on Si(001): The Bi-dimer line
- Theoretical Approach: Ab initio calculations
- Electronic properties of Fe atoms on the Bi-H/Si(001)
- Magnetic properties of Fe atoms on Bi-H/Si(001)
- Summary and conclusions

Bi nanolines on Si(001): STM images

Taken from the J. Owen webpage[1]





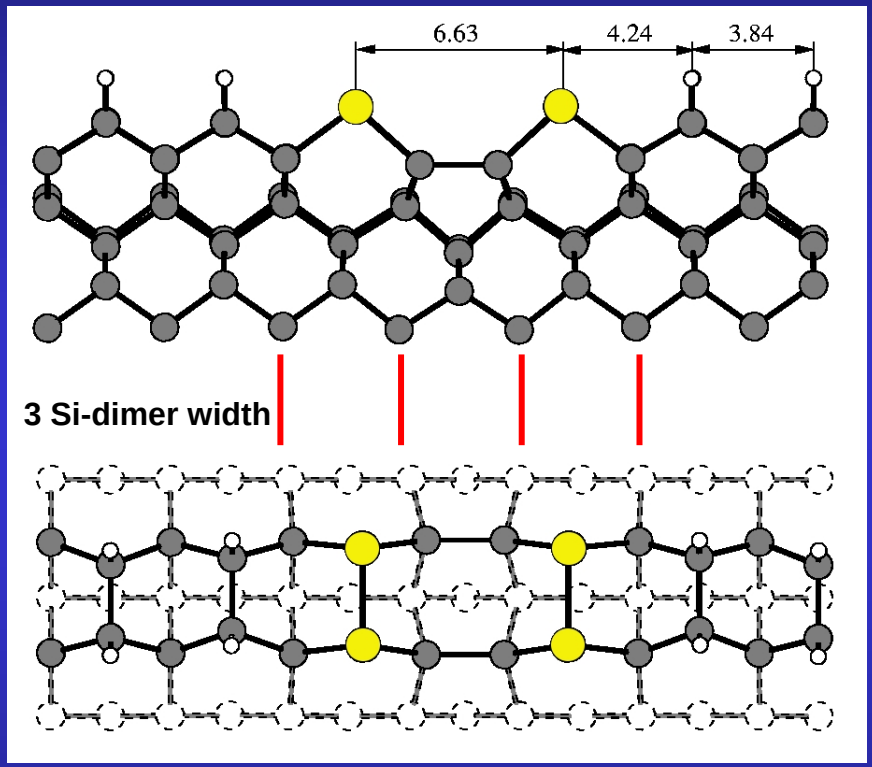


- Bi lines are very long (> 500 nm) but only 1.5 nm wide (4 Si dimer width), perfectly straight and essentially free of kink and defect
- They form after Bi deposition at a substrate temperature above 500 °C, followed by annealing
- They are insulating and chemically inert, being resistant to the attack of atomic hydrogen, O_2 and O_3
- Thus, these lines are very promising to pattern one-dimensional atomic structures by direct atomic deposition

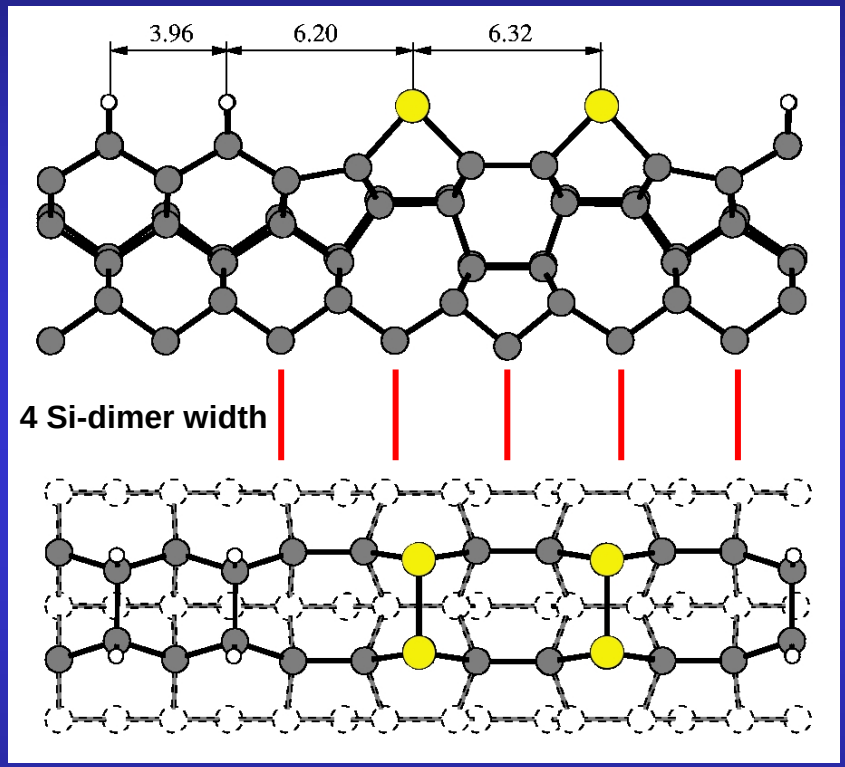
Owen et al., Phys. Rev. Lett. 88, 226104 (2002) , Surf. Sci. Lett. 499, L124 (2002)
(1) http://homepage.mac.com/jhgowen

Atomic geometry of Bi nanolines on H/Si(001)

Miki Model



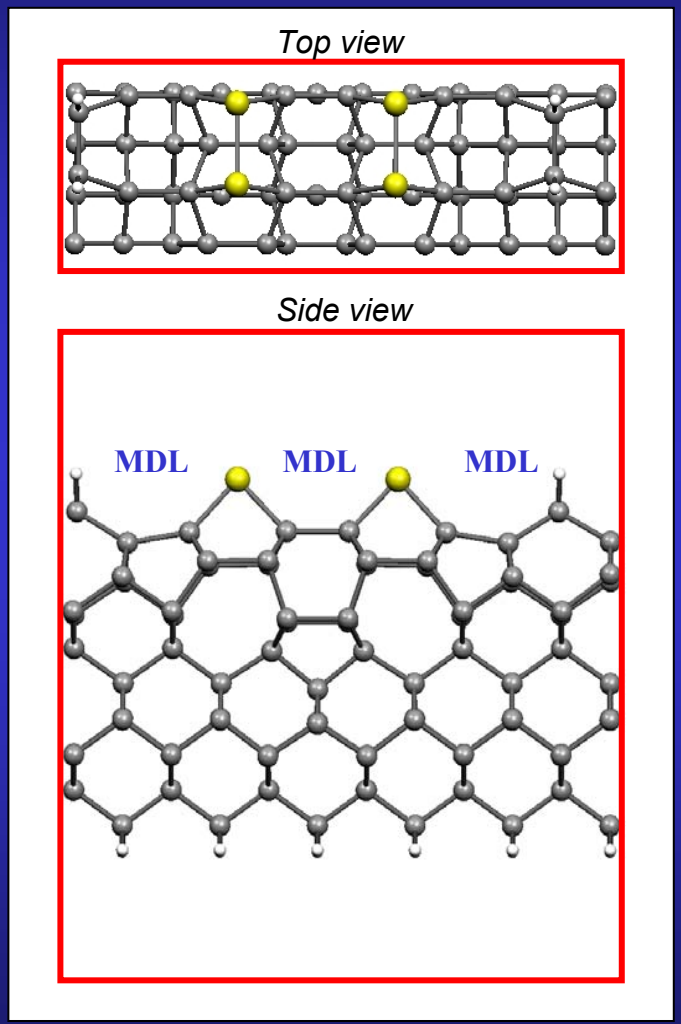
Haiku Model (-0.57 eV/dimer)



- After hydrogenation, hydrogen acts as a mask over the surrounding silicon, leaving the Bi lines clean
- The Haiku model has a Bi line spacing of 4 Si dimers which agrees well with the STM images
- Ab initio calculations show that the Haiku model is more stable than the Miki model by 0.6 eV/dimer

Miwa et al., Nanotechnology 16, 2427 (2005)

Theoretical Method

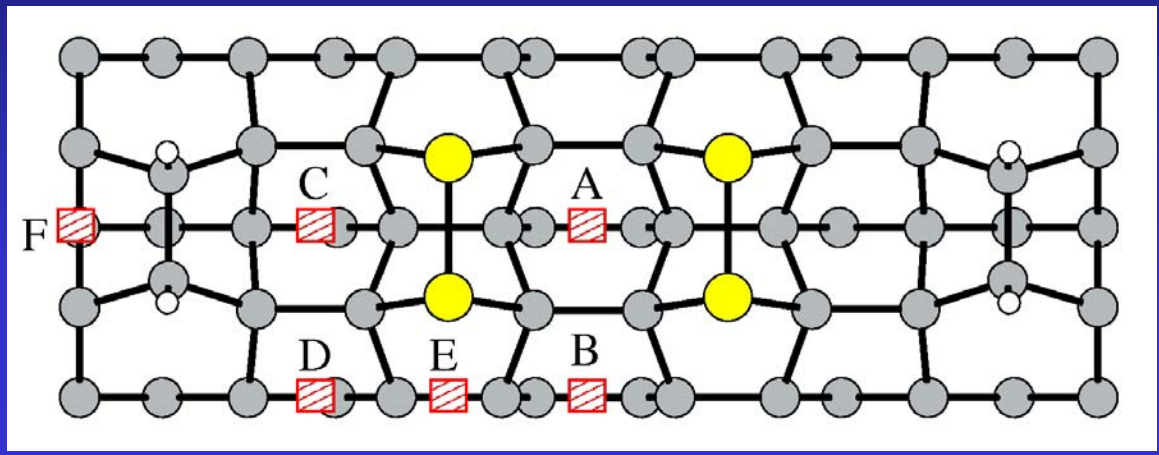


MDL=missing dimer lines

- Spin-polarized density functional calculations (DFT) within the Local Spin Density Approximation (LSDA)
- Noncollinear treatment of magnetization
  The direction of magnetization is a continuous variable of position which is allowed to relax simultaneously with the geometry
- Norm-conserving pseudopotentials, including pseudocore corrections
- Basis set of localized numerical pseudoatomic orbitals (DZP, according to the SIESTA method)
- 2×6 surface unit cell with 10 monolayers (148 atoms) and a vacuum region of 11 Å
- Four special k points along the Bi-dimer line are use to sample the Brillouin zone
- The topmost eight monolayers are fully relaxed until forces at each atoms become smaller than 0.05 eV/Å
- Spin-orbit interactions are not considered

Fe adsorption on the Bi lines structure

Six adsorption sites for the Fe atoms on the Bi-dimer structures are investigated



Sites	ΔE (eV)	E_b (eV)	m (μ_B/Fe)	*CN*
A	0.13	5.83	1.83	6
C	0.00	5.97	1.53	7
B	0.35	5.62	1.63	6
D	0.12	5.85	1.27	7
E	0.82	5.15	1.99	8
F	1.07	4.90	1.95	7

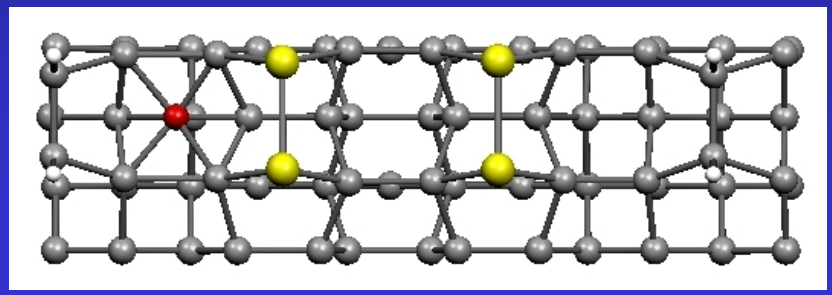
E_b = binding energy
m = magnetization
CN = coord. number

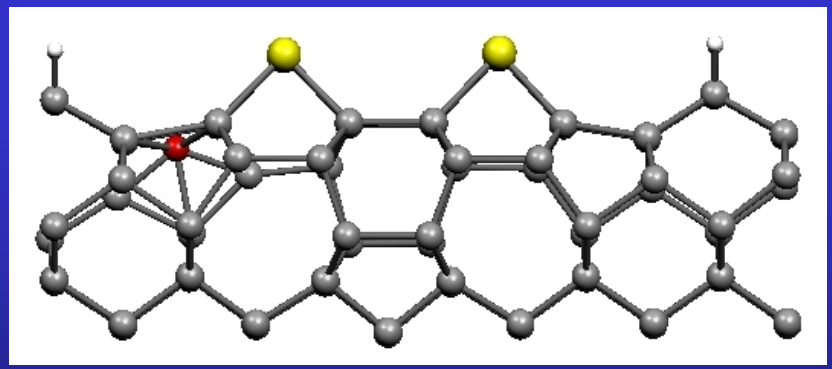
The missing dimer lines (MDLs) are the energetically favorable positions for the Fe adatoms

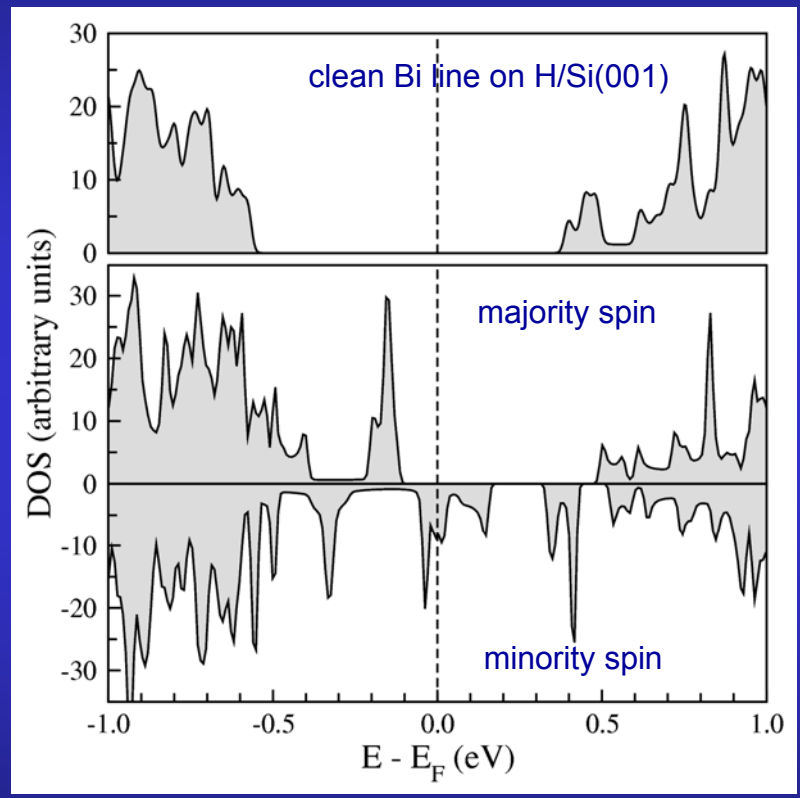
The Fe adsorption at the most stable site (C)

The Fe adatom tends to increase the number of Fe-Si bonds occupying an interstitial subsurface position, about 0.5 Å below the topmost Si atoms, becoming sevenfold coordinated

$d_{Fe\text{-}Si}$ ~ 2.2 – 2.5 Å

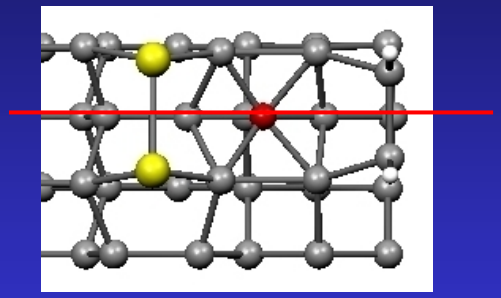


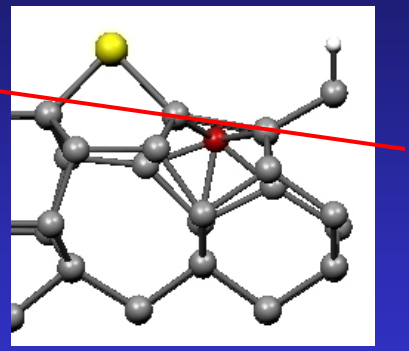




Along the Bi-dimer lines we find a magnetic half metal behavior : The majority spin channel behaves as a semiconductor with a band gap of about 0.6 eV and the minority spin channel behaves as metal

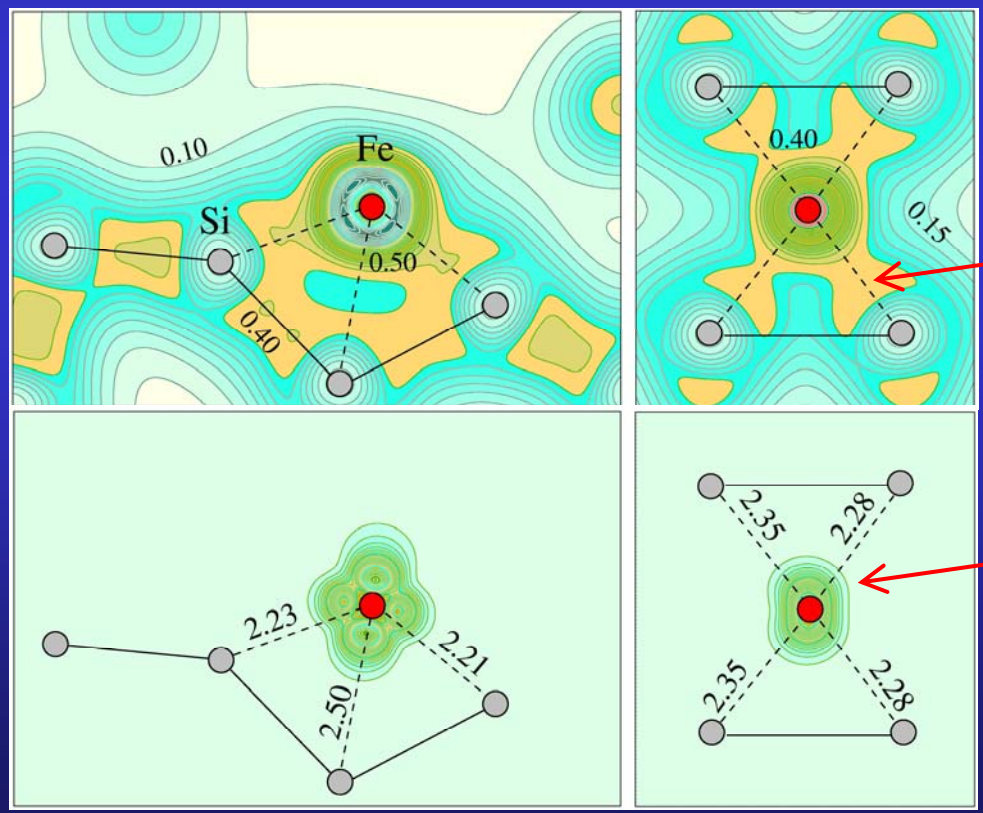
Total charge density for the Fe adatom





The high coordination of Fe adatoms suggests that orbital magnetization might be small or even be quenched

Fe	m_S (μ_B)	m_{ORB} (μ_B)
atom	4	2
surface	2.5-3.0	0.07-0.12
bulk	2.2	0.05



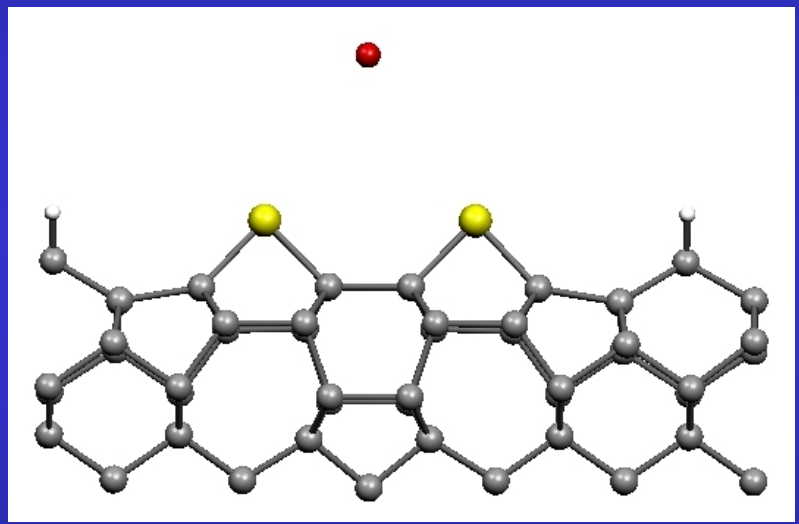
Total charge density contour plots indicate metallic Fe-Si bonds

Spin density contour plots indicate that the magnetization is concentrated at the Fe atoms

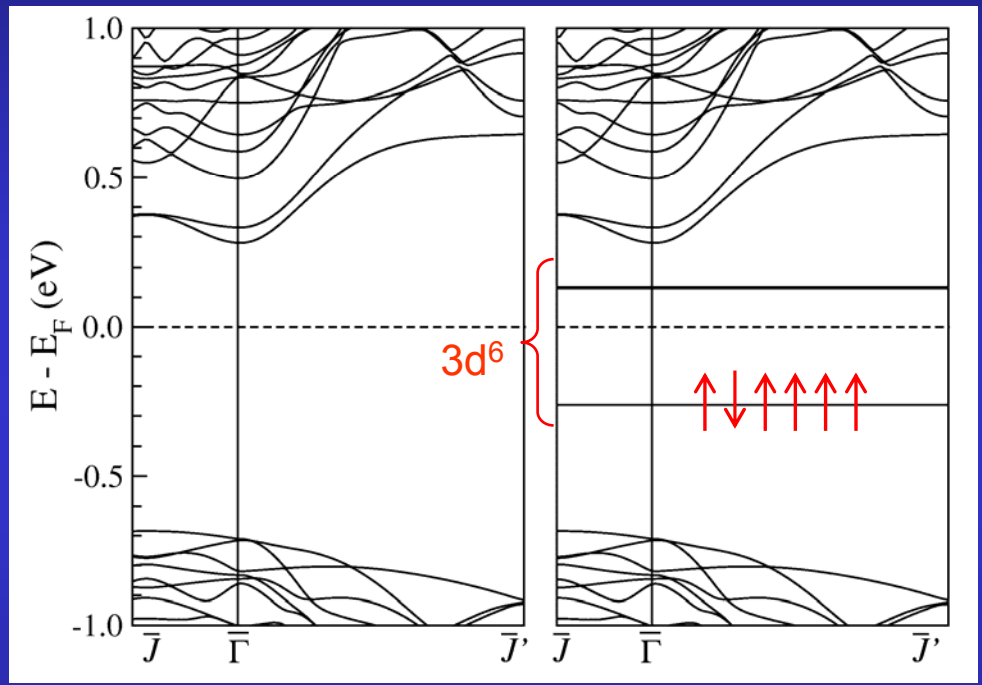
Different Si-Fe bond distances suggest a highly anisotropic Fe environment

Fe adsorption on Bi nanolines

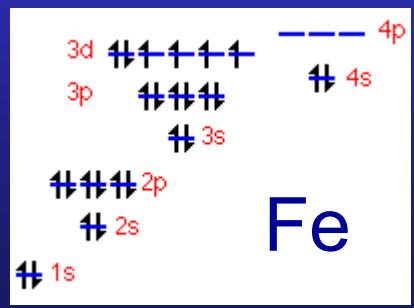
Initially, we fix the Fe atom 5 Å above the surface in order to determine the localization of the Fe 3d atomic orbital



Minority Spin Majority Spin



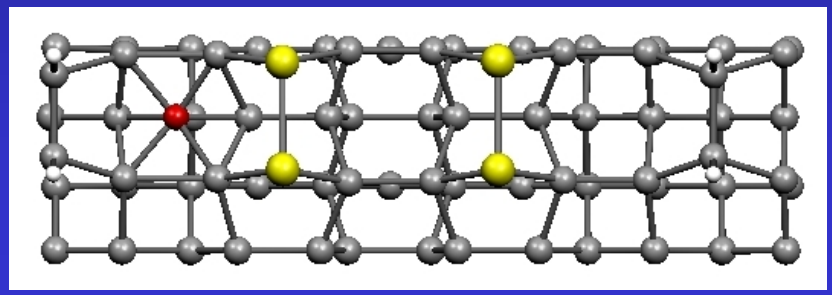
$$m_S = 2S\,\mu_B = 4.0\,\mu_B$$



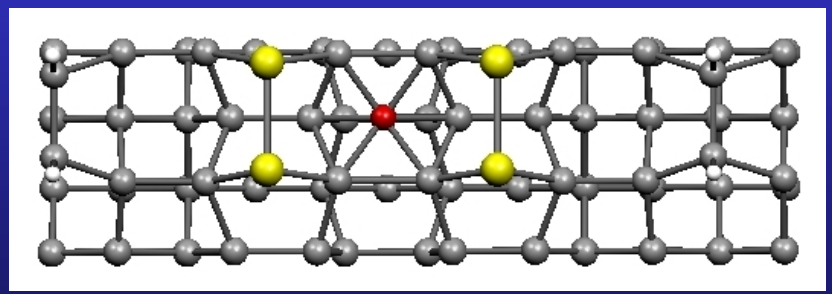
Fe adatom at C and A sites

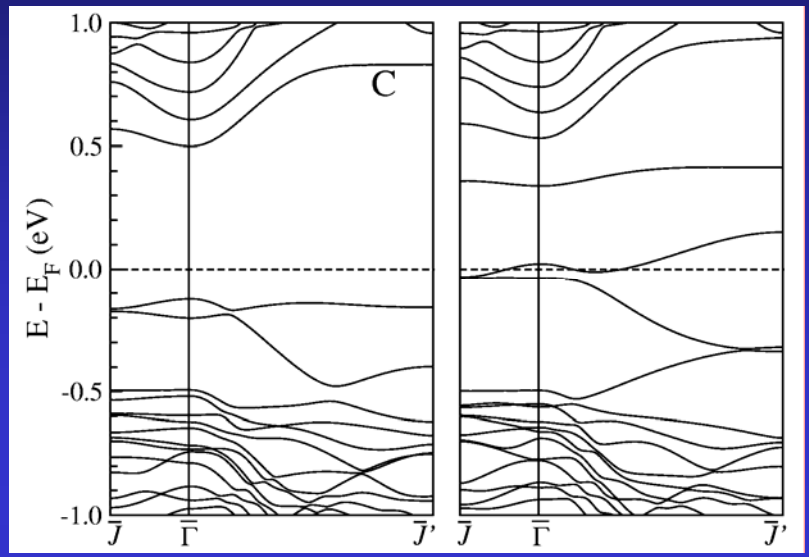
When the Fe atom is adsorbed between Bi dimers is observed a magnetic half-metal behavior

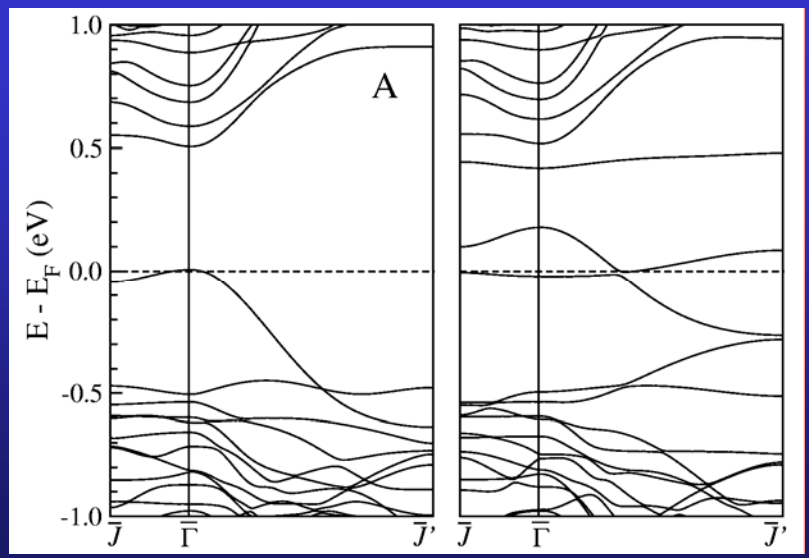
E_0 , $m = 1.53\ \mu_B$



$E_0 + 0.13$ eV, $m = 1.83\ \mu_B$



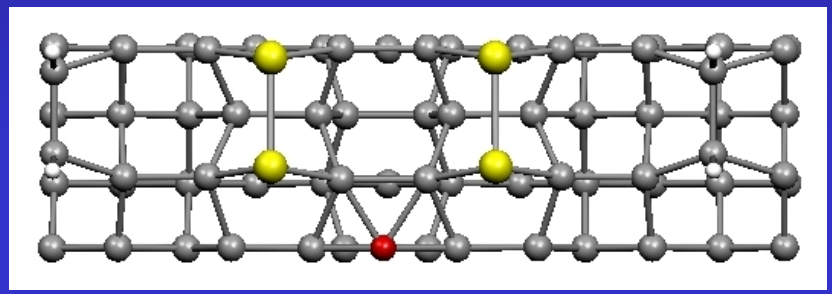




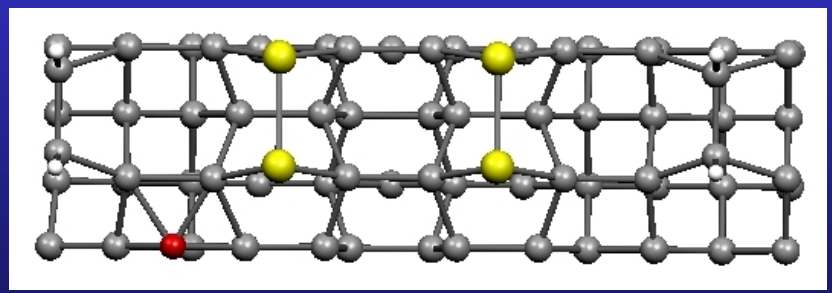
Fe adatom at B and D sites

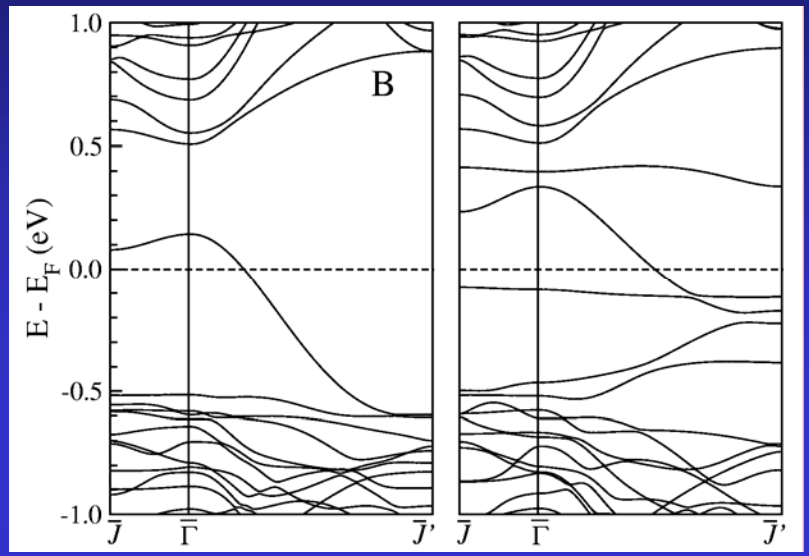
When the Fe atom is adsorbed between Bi dimers of the same line both spin channels show a metallic character

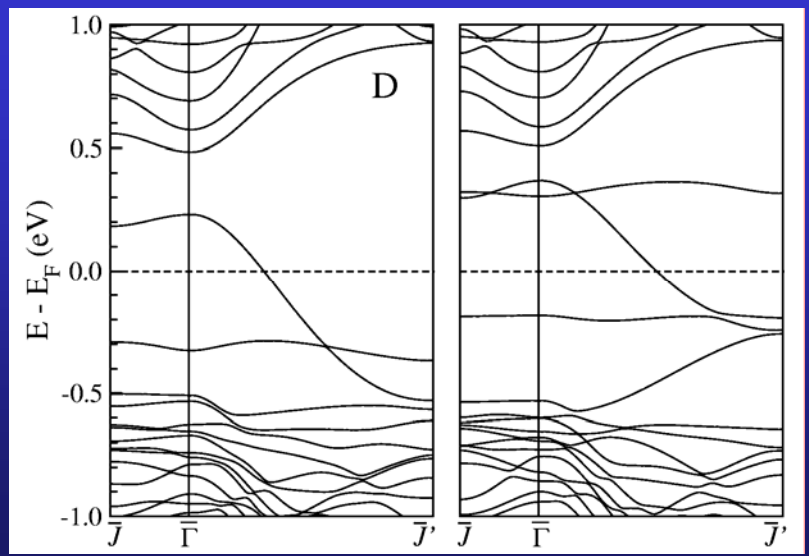
E_0 + 0.35 eV, m = 1.63 μ_B



E_0 + 0.12 eV, m = 1.27 μ_B





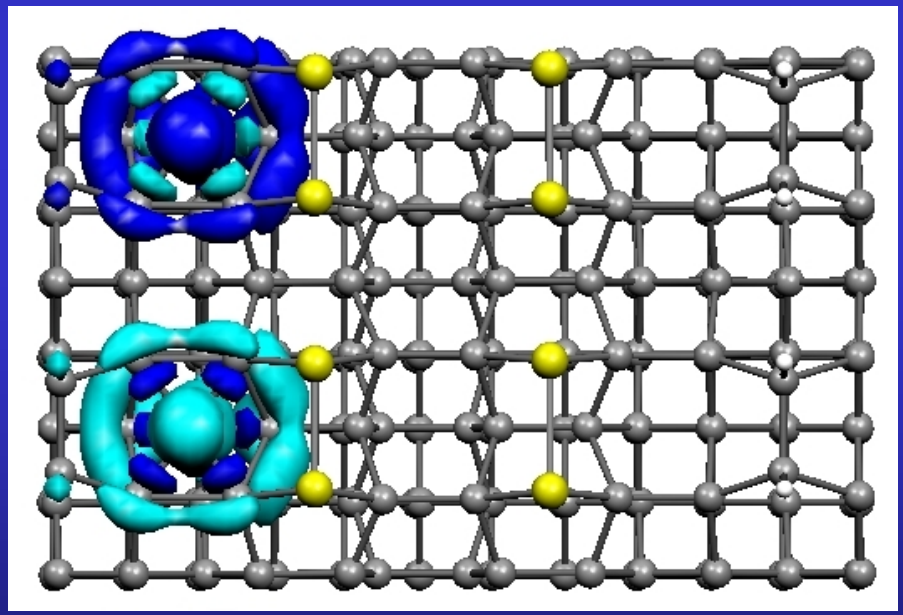


Magnetic Ordering of Fe adatoms

The stable magnetic ordering of the 1D Fe array on the Bi nanolines is calculated by doubling the supercell (298 atoms !)

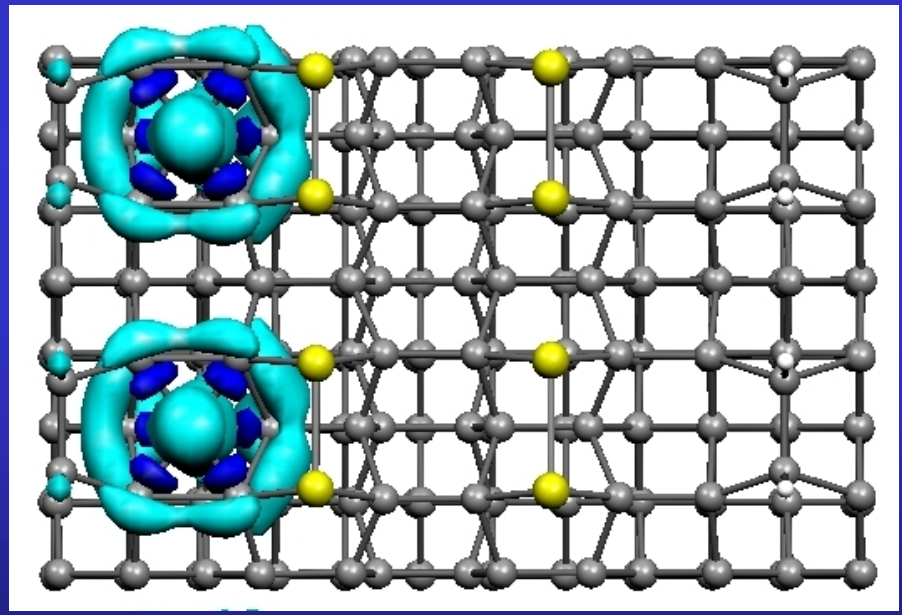
$m = 0$

antiferromagnetic ordering (AFM)



$m = 1.61\ \mu_B / Fe$

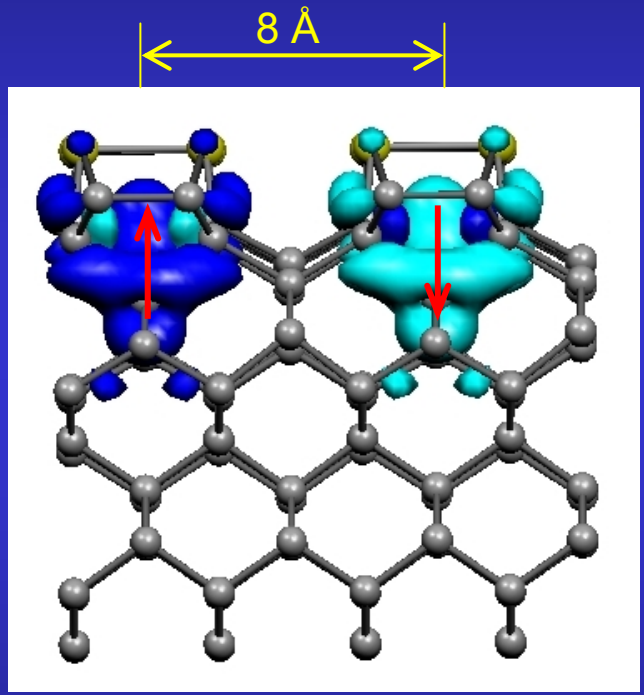
ferromagnetic ordering (FM)



Spin density isosurfaces ($\rho^{\uparrow} - \rho^{\downarrow} = 0.04$ [$eV/Å^3$])

Magnetic Coupling of Fe adatoms

The strength of the magnetic coupling between Fe atoms is estimated taken the difference in energy between the ferromagnetic (FM) and antiferromagnetic (AFM) ordering



$$J_{Fe-Fe} = E_{FM} - E_{AFM} = 14.4 \text{ meV}$$

It is possible that Fe adatoms exhibit magnetic anisotropy like thin films of amorphous Fe-Si alloys ?

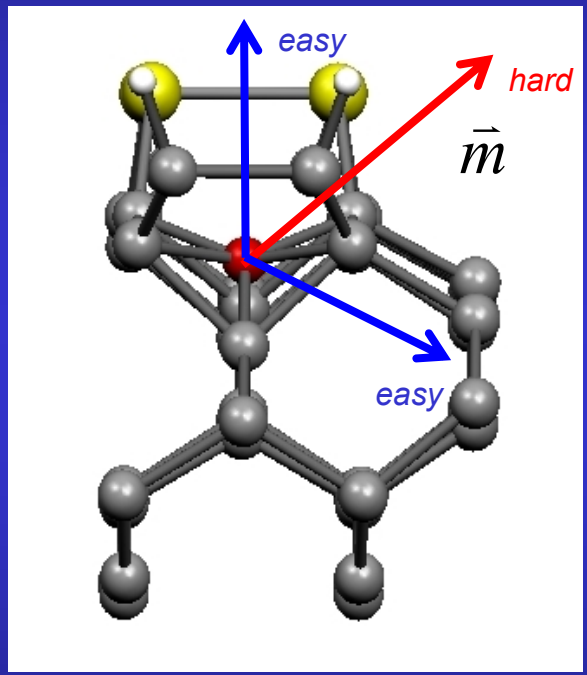
Diaz et al., IEEE Trans. Mag., 38, 2811 (2002)

Magnetic Fe-Si amorphous alloys prepared as thin films usually have a well defined magnetization axis (easy axis)

The magnetic anisotropy should come from magnetic dipolar interaction originated in the adsorption site due to the structural anisotropy and from spin-orbit interactions.

Giant Magnetic Anisotropy

We estimate a lower limit for the magnetic anisotropy energy (E_{MA}) by taking the difference in energy between the magnetization pointing in a direction of low energy (easy axis) toward one of high energy (hard axis) by noncollinear spin calculations

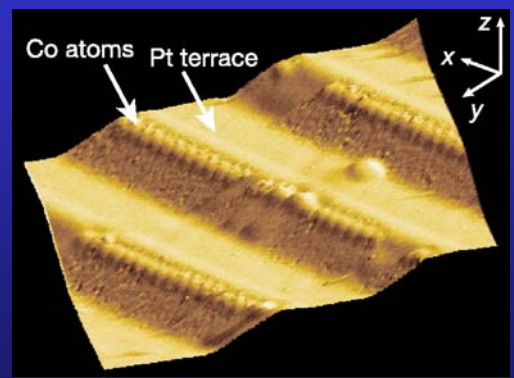


easy axis $\theta \approx 0,\ 117^o$

hard axis $\theta \approx 50^o$

$E_{MA} \approx E_{total}(hard) - E_{total}(easy) = 3.6\ meV/atom$

The MAE of Fe adatoms on the Bi line has the same order of magnitud than those measured for the Co chains on vicinal steps of Pt(997) ~ 2 meV/atom



Gambardella.et al., Nature 416, 301 (2002)

Summary and Conclusions

- Fe atoms occupy highly coordinated subsurface positions at the missing dimer line (beside the Bi lines), allowing the forming 1D atomic arrays
- At the most stable positions (the C site), the Fe array couples antiferromagnetically with a weak exchange coupling ($J_{Fe\text{-}Fe}$=14 meV)
- We find that the structural anisotropy of the Fe adatom sites induces a large magnetic anisotropy estimated in 3 meV/atom, which originates in the magnetic dipolar interactions
- According to our results, self-assembled Bi lines on H/Si(001) may have potential applications in the patterning of 1D atomic arrays for magnetic devices

For more details please see: Appl. Phys. Lett. 89, 093105 (2006)