

Ab initio methods in solid state physics

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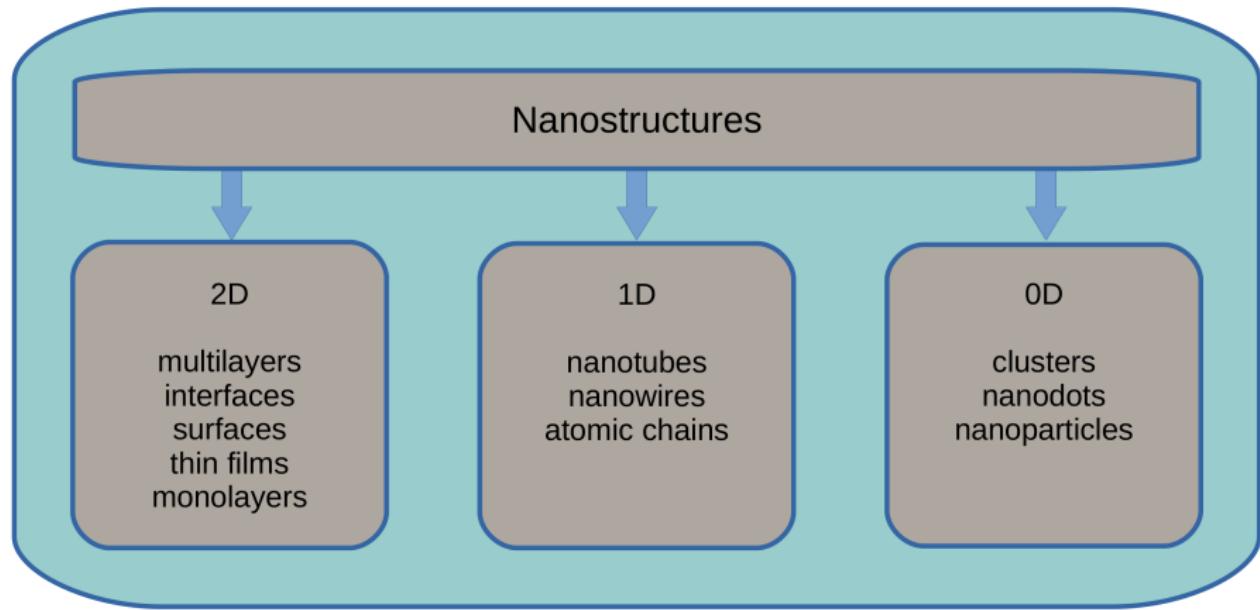
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- 3 Electronic states in crystals
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Nanostructures

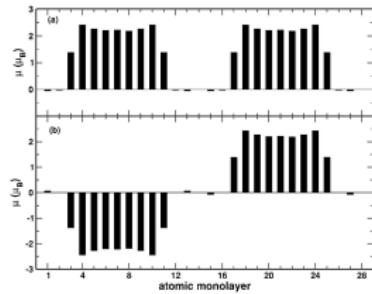
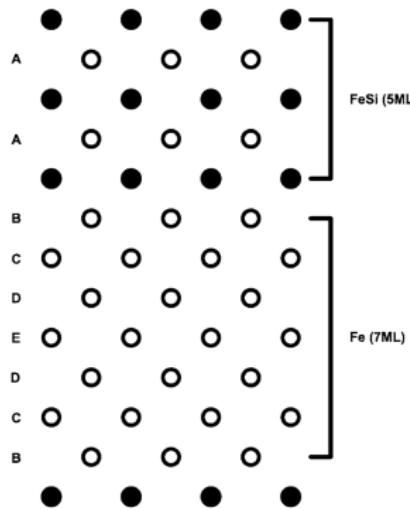
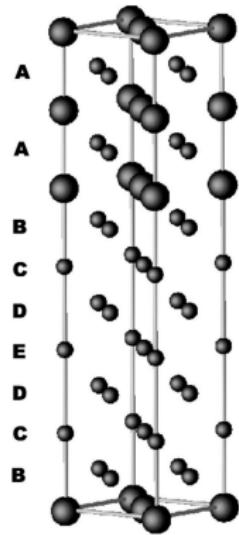
Nanostructure - material with a reduced size (< 100 nm) in 1D, 2D or 3D.



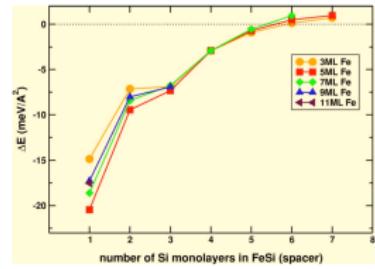
Multilayers FeSi/Fe

P. T. Jochym, K. Parlinski, and A.M. Oleś, Phys. Rev. B **73**, 224411 (2006)

FeSi(N monolayers)/Fe(M monolayers)



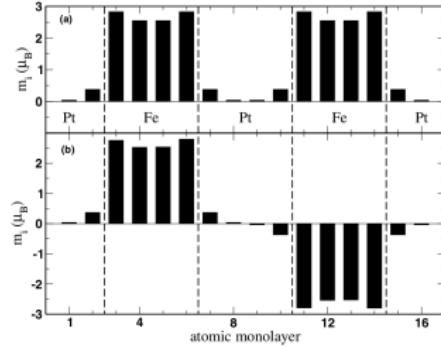
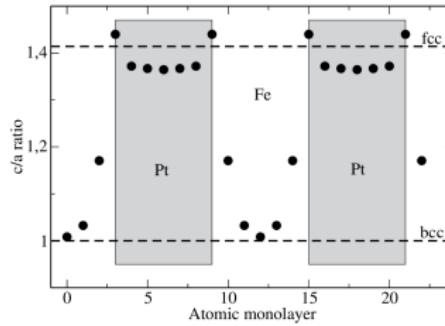
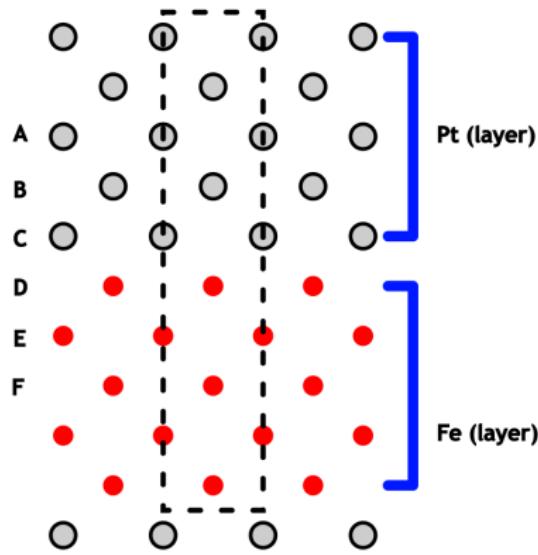
$$\Delta E = E_{AF} - E_{FM}$$



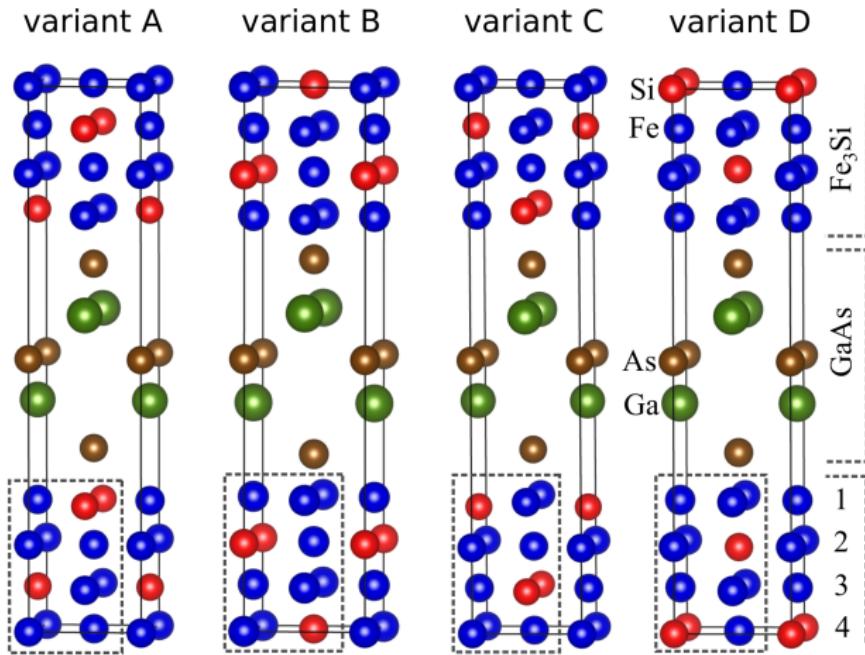
Multilayers Pt/Fe

P. T. Jochym, K. Parlinski, and A.M. Oleś, Eur. Phys. J. B **61**, 173 (2008)

Pt(N monolayers)/Fe(M monolayers)

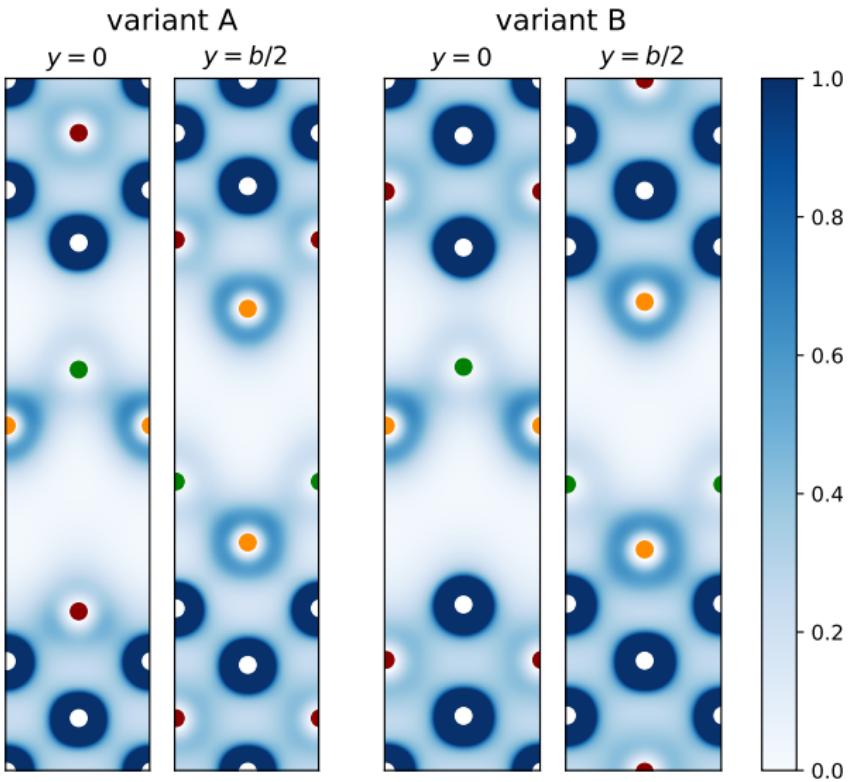


Multilayers Fe₃Si/GaAs

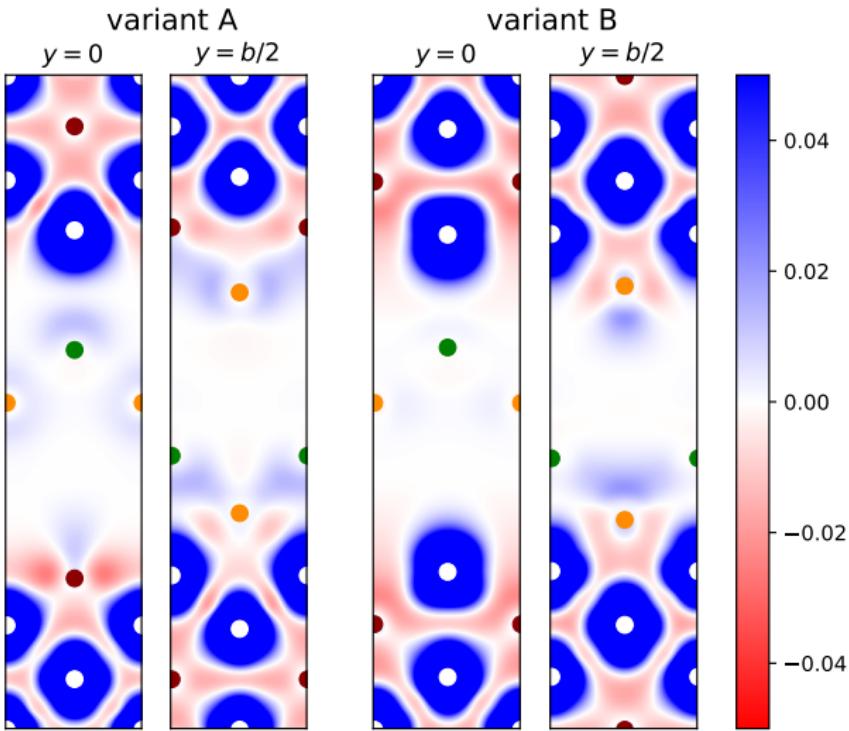


O. Sikora, J. Kalt, M. Sternik, A. Ptok, P. T. Jochym, J. Łazewski, K. Parlinski, P. Piekarz, I. Sergueev, H.-C. Wille, J. Herfort, B. Jenichen, T. Baumbach, and S. Stankov, Phys. Rev. B **99**, 134303 (2019)

Multilayers Fe₃Si/GaAs – charge density

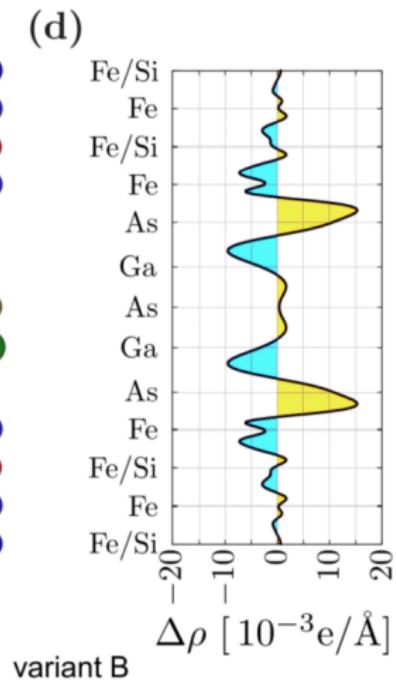
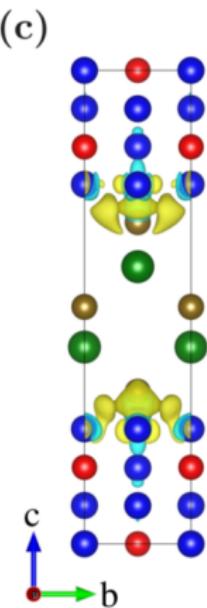
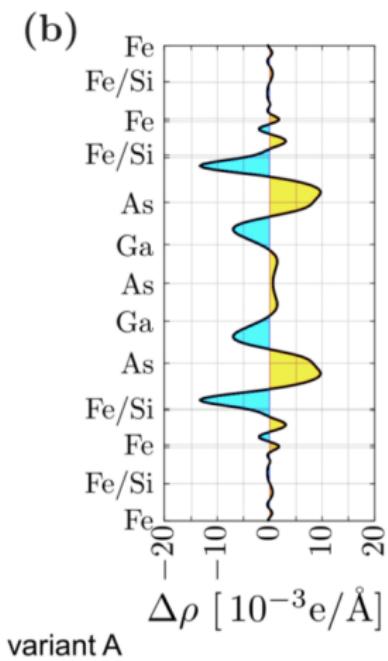
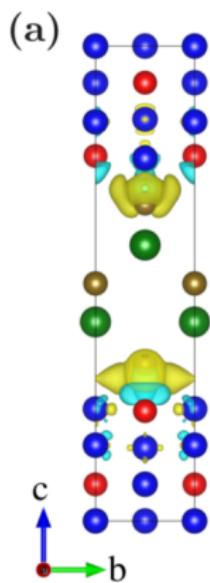


Multilayers Fe₃Si/GaAs – magnetization density

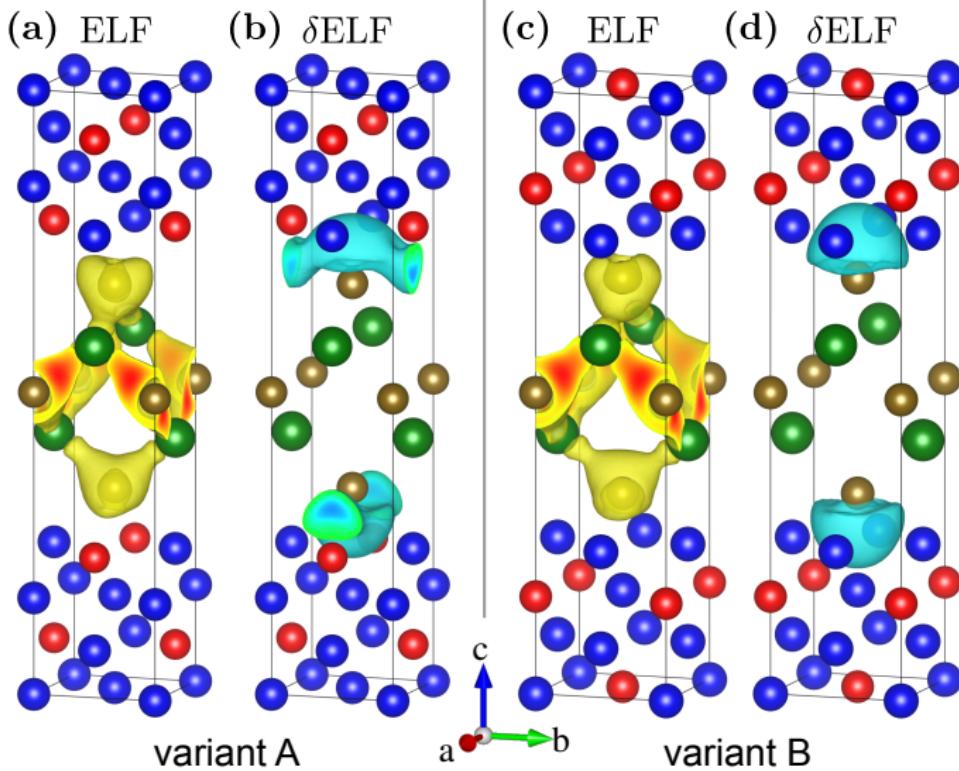


Multilayers Fe₃Si/GaAs – charge transfer

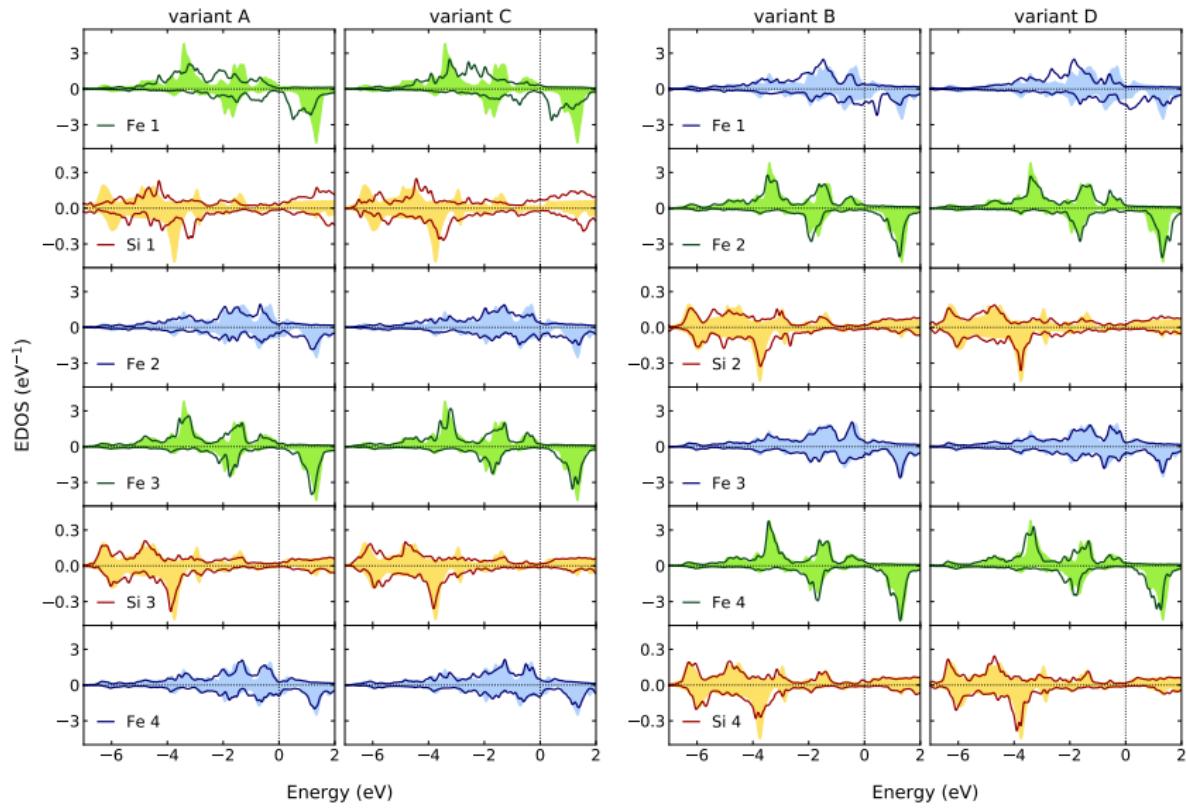
$$\Delta\rho = \rho_{\text{FeSi}/\text{GaAs}} - \rho_{\text{FeSi/vac}} - \rho_{\text{vac/GaAs}} \quad (1)$$



Multilayers Fe₃Si/GaAs – ELF



Multilayers Fe₃Si/GaAs – electron density of states



Multilayers Fe₃Si/GaAs – magnetic anisotropy

TABLE III. Spin polarization at the Fermi energy for each layer and the total value at the interface. In bold we denote values for pure Fe layers (bulk value -0.53) and the remaining values are for the mixed Fe-Si layers (bulk value 0.48). The total polarization in the bulk Fe₃Si is equal to -0.41.

| Layer | Variant A | Variant B | Variant C | Variant D |
|--------------------------|--------------|--------------|--------------|--------------|
| 1 | -0.60 | -0.44 | 0.21 | -0.76 |
| 2 | -0.51 | 0.32 | -0.38 | -0.02 |
| 3 | 0.14 | -0.15 | 0.26 | -0.24 |
| 4 | -0.69 | 0.72 | -0.39 | 0.61 |
| Total Fe ₃ Si | -0.52 | -0.23 | -0.26 | -0.49 |

Spin polarization

$$P = \frac{N_{\uparrow}(E_F) - N_{\downarrow}(E_F)}{N_{\uparrow}(E_F) + N_{\downarrow}(E_F)}. \quad (2)$$

Magnetic anisotropy energy (MAE)

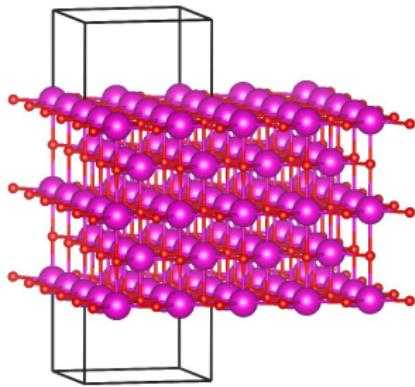
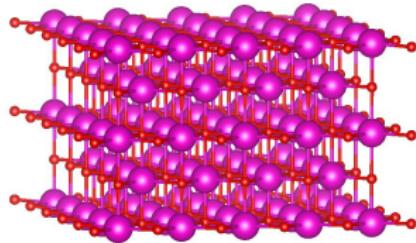
$$\Delta E = E[h_2 k_2 l_2] - E[h_1 k_1 l_1]. \quad (3)$$

TABLE II. Magnetic anisotropy energy (MAE), in meV per primitive unit cell, calculated for different Fe₃Si/GaAs interface variants and compared with the values obtained for cubic and tetragonally deformed Fe₃Si crystal. The total energies are calculated for spins aligned along various directions in the crystallographic cell of Fe₃Si.

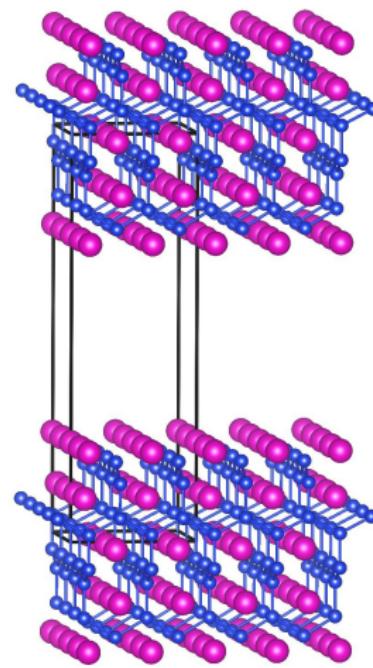
| MAE (meV/p.u.c.) | Interface variants | | | | Bulk Fe ₃ Si | |
|-------------------------|--------------------|-------|-------|-------|-------------------------|------------|
| | A | B | C | D | Cubic | Tetragonal |
| $E_{[100]} - E_{[001]}$ | 0.10 | 0.17 | 0.10 | -0.57 | 0.00 | -0.26 |
| $E_{[110]} - E_{[001]}$ | -9.28 | -7.38 | -8.03 | -1.25 | 0.01 | -0.27 |
| $E_{[110]} - E_{[100]}$ | -9.38 | -7.55 | -8.13 | -0.68 | 0.01 | -0.01 |

Surfaces

$\text{EuO}(001)$



$\text{EuSi}_2(001)$



Surface and interface energy

The surface energy of the solid X can be obtained from the following formula

$$\sigma_X = \frac{1}{2A_{\text{surf}}} (E_X^{\text{slab}} - n_X \varepsilon_X^{\text{bulk}}), \quad (4)$$

where E_X^{slab} is the total energy of the slab, $\varepsilon_X^{\text{bulk}}$ is the energy of the bulk crystal per one atom, n_X is the number of atoms in the slab, and A_{surf} is the area of the surface.

In a similar way we can calculate the energy of the interface build of the X and Y crystals

$$\gamma_{XY} = \frac{1}{2A_{\text{int}}} [E_{XY} - (n_X \varepsilon_X^{\text{bulk}} + n_Y \varepsilon_Y^{\text{bulk}})], \quad (5)$$

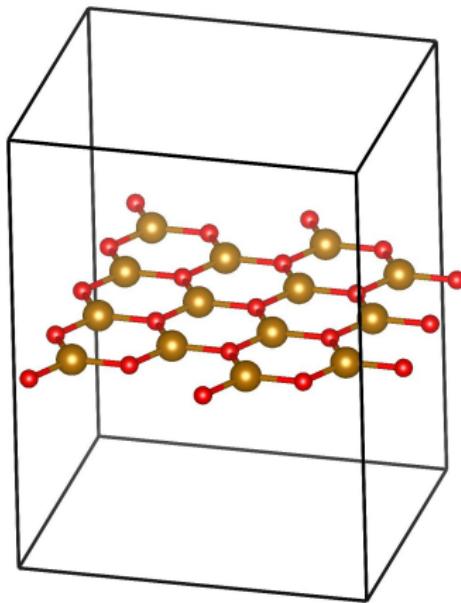
where E_{XY} is the total energy of the XY interface.

The work of separation is defined as the energy required to separate an interface into two semi-infinite bulks with free surfaces

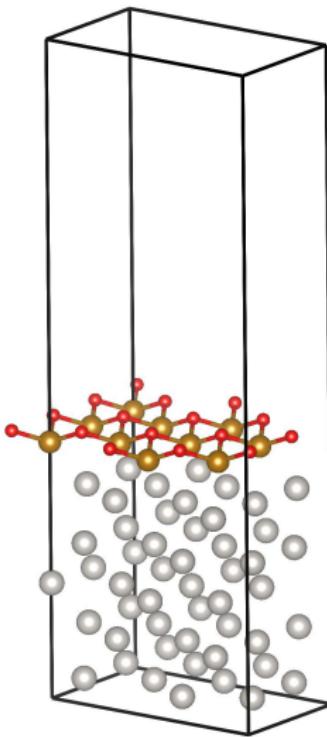
$$W_{\text{sep}} = \sigma_X + \sigma_Y - \gamma_{XY}. \quad (6)$$

Monolayers and thin films FeO/Pt

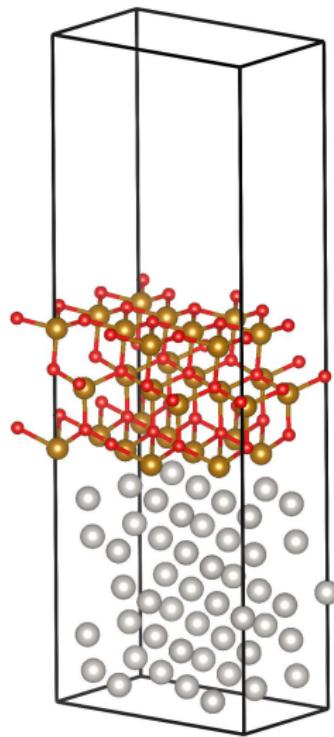
1ML FeO(111)



1ML FeO/Pt(111)



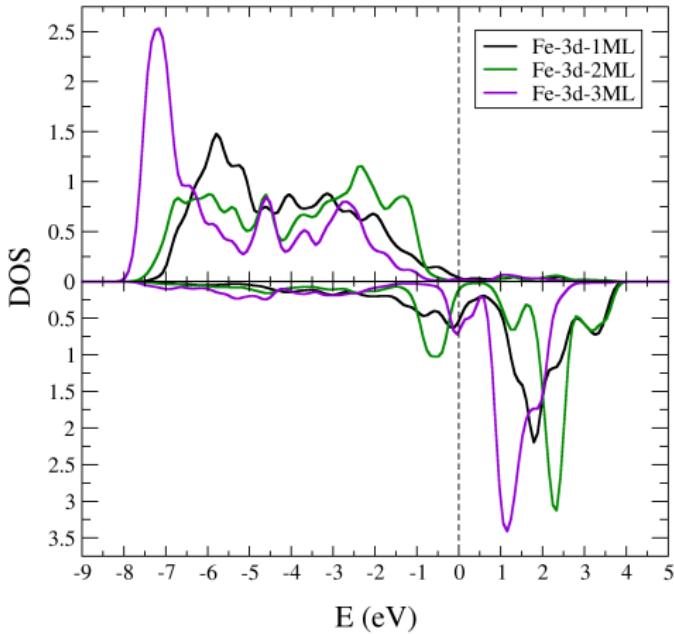
3ML FeO/Pt(111)



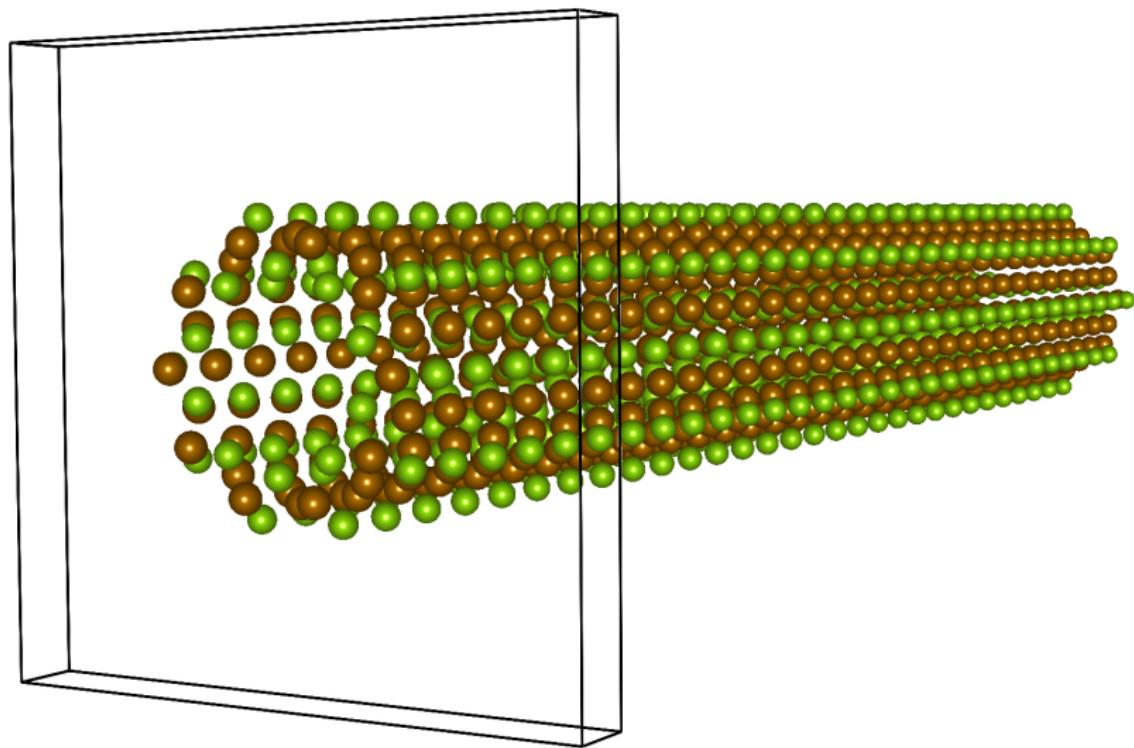
Monolayers and thin films FeO/Pt

Magnetic moments

| Atom | 3ML | 2ML | 1ML |
|------|-------|-------|-------|
| Fe3 | 3.816 | | |
| O3 | 0.102 | | |
| Fe2 | 3.525 | 3.835 | |
| O2 | 0.100 | 0.098 | |
| Fe1 | 3.556 | 3.544 | 3.771 |
| O1 | 0.030 | 0.107 | 0.069 |
| Pt1 | 0.020 | 0.036 | 0.165 |
| Pt2 | 0.022 | 0.024 | 0.012 |

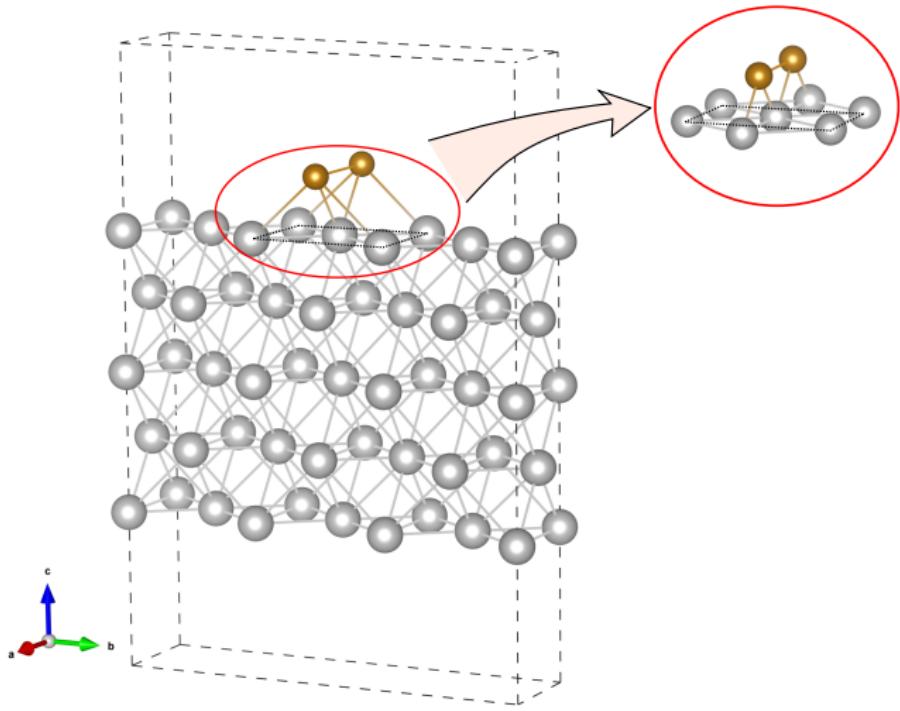
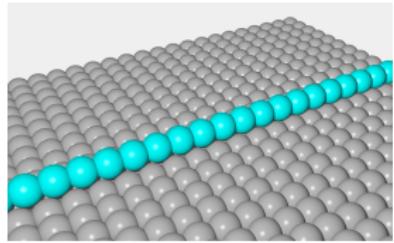


Nanotubes

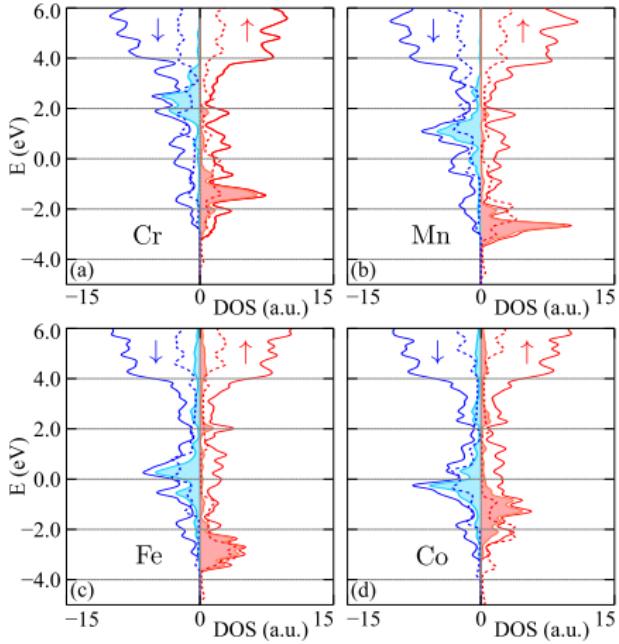
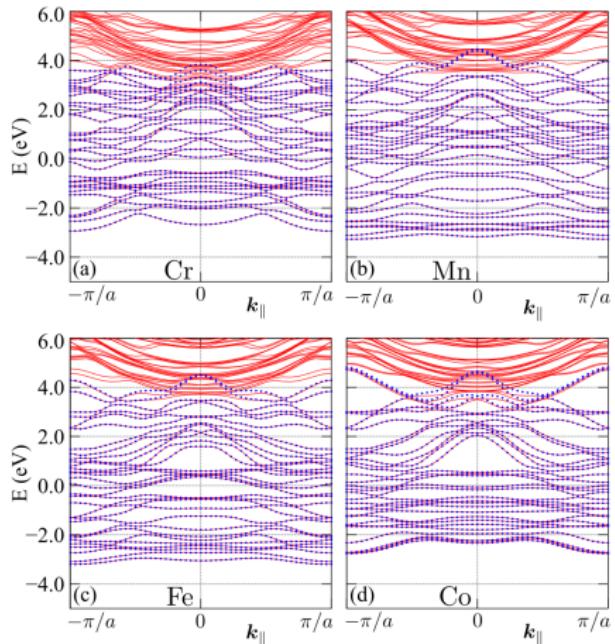


Monoatomic chains

Fe/Pb(110)

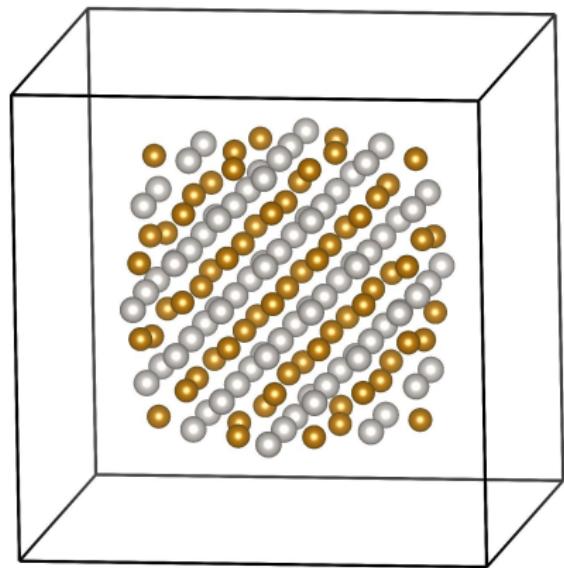
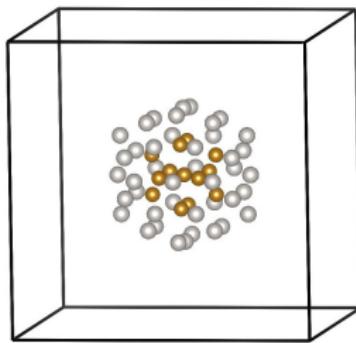
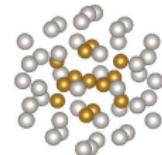
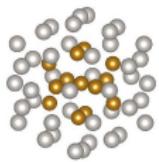
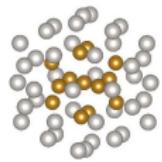


Monoatomic chains



A. Kobiałka, P. Piekarcz, A. M. Oleś, and A. Ptok,
Phys. Rev. B **101**, 205143 (2020)

Nanoparticles



Nanoparticles

