

Ab initio methods in solid state physics

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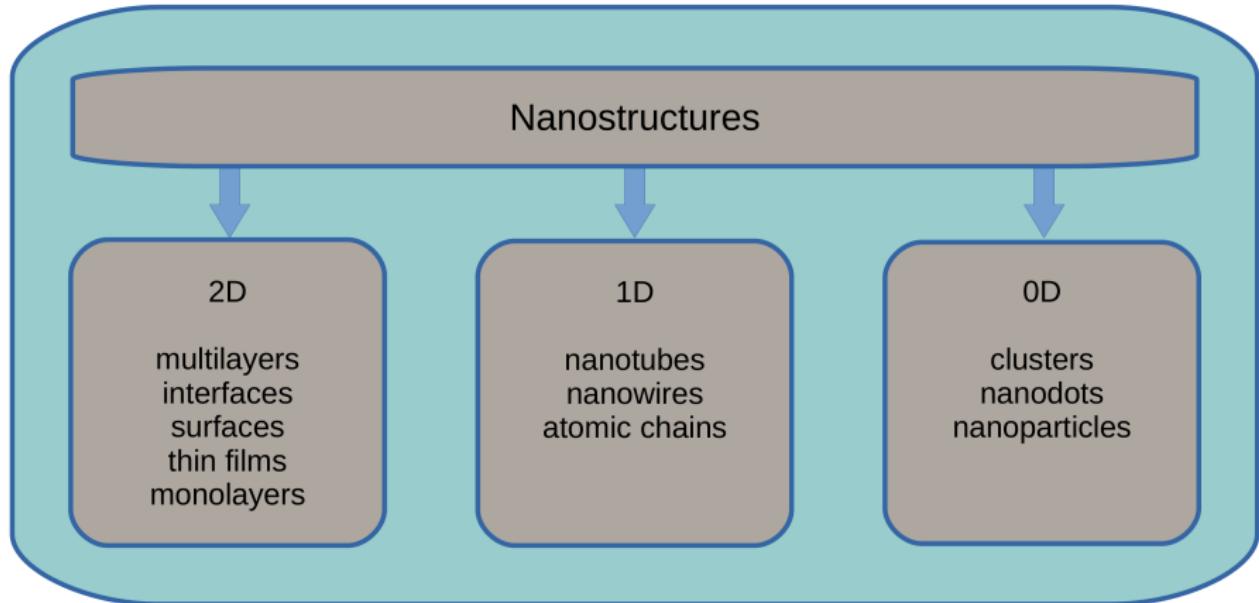
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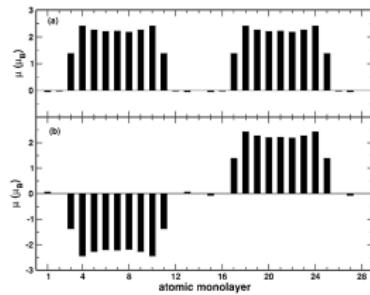
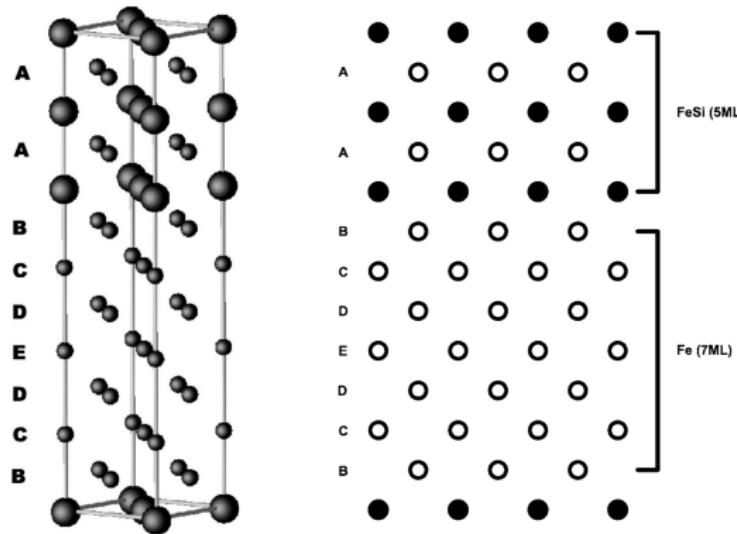
Nanostructure



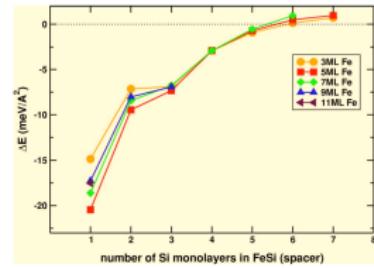
Multilayers FeSi/Fe

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

FeSi(N monolayers)/Fe(M monolayers)



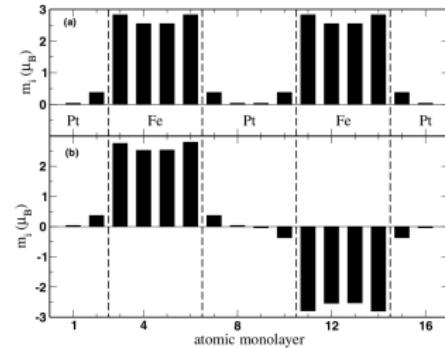
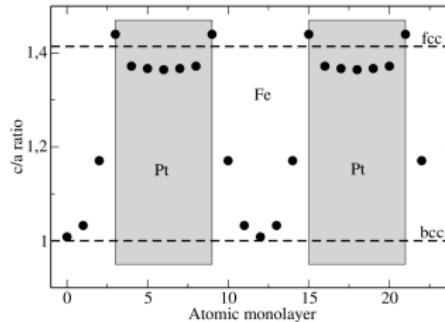
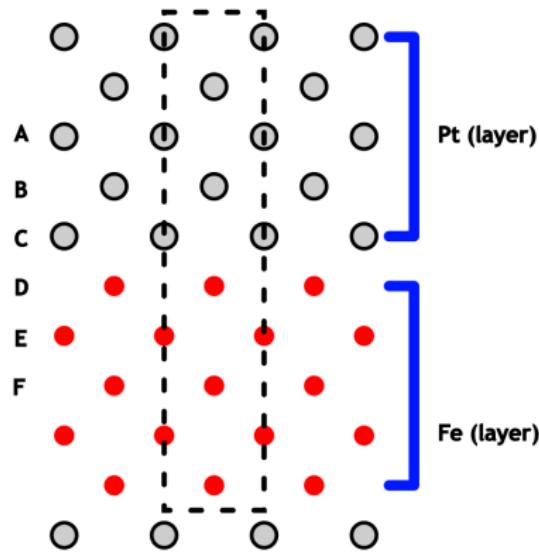
$$\Delta E = E_{AF} - E_{FM}$$



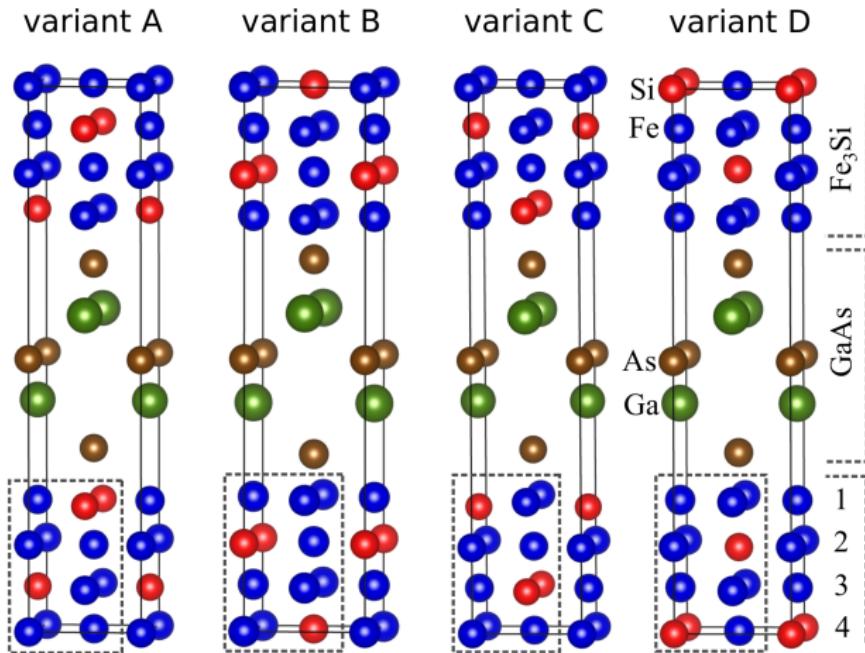
Multilayers Pt/Fe

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

Pt(N monolayers)/Fe(M monolayers)

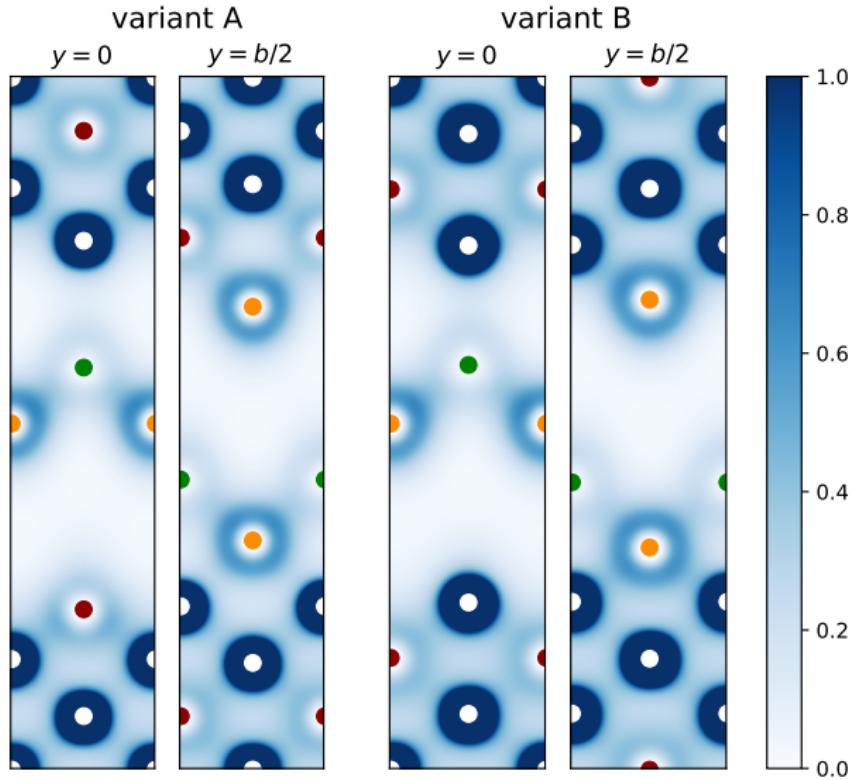


Multilayers Fe₃Si/GaAs

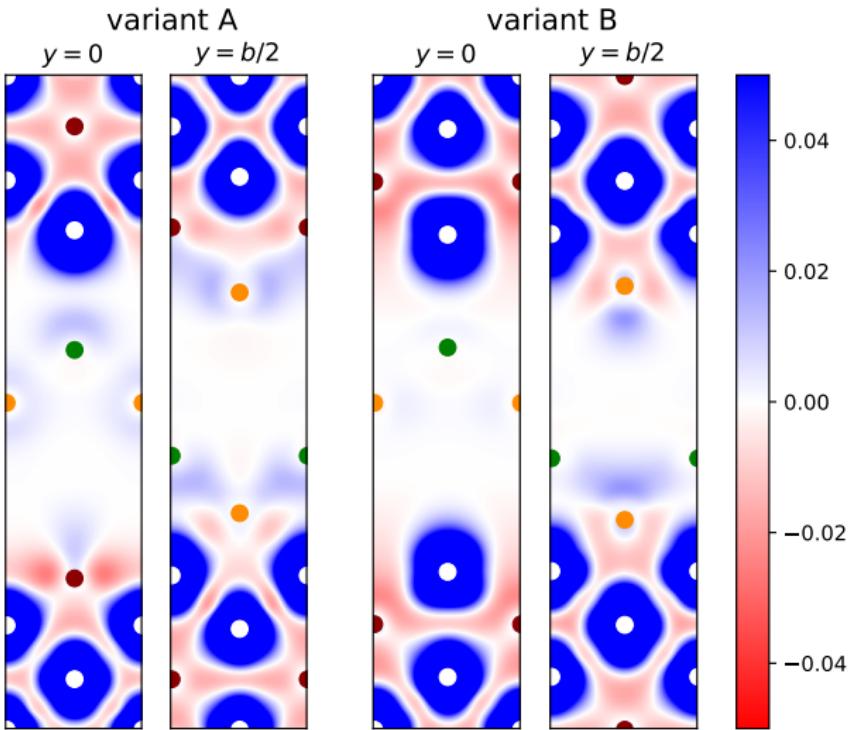


O. Sikora, J. Kalt, M. Sternik, A. Ptok, P. T. Jochym, J. Łazewski, K. Parlinski, P. Piekarz, I. Sergueev, H.-C. Wille, J. Herfort, B. Jenichen, T. Baumbach, and S. Stankov, Phys. Rev. B **99**, 134303 (2019)

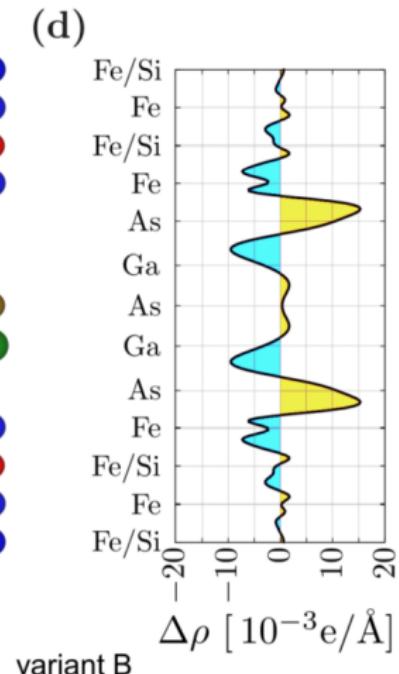
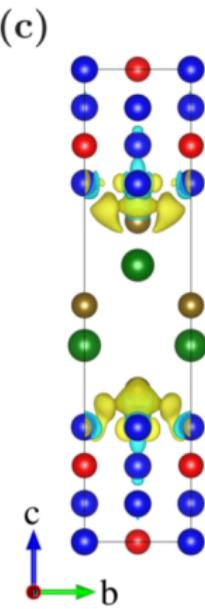
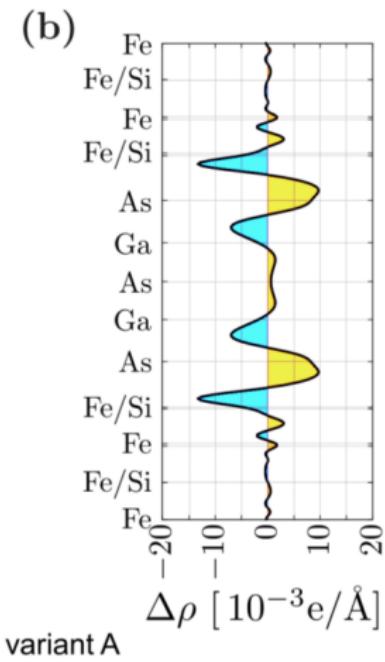
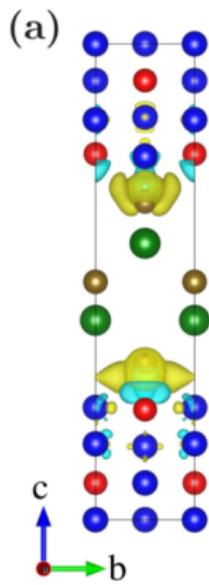
Multilayers Fe₃Si/GaAs – charge density



Multilayers Fe₃Si/GaAs – magnetization density



Multilayers Fe₃Si/GaAs – charge transfer



Electron localization function (ELF)

The electron localization function is obtained from the equation

$$\text{ELF} = \frac{1}{1 + \alpha^2}, \quad (1)$$

where α is the dimensionless parameter

$$\alpha = \frac{\tau - \tau^w}{\tau^u}, \quad (2)$$

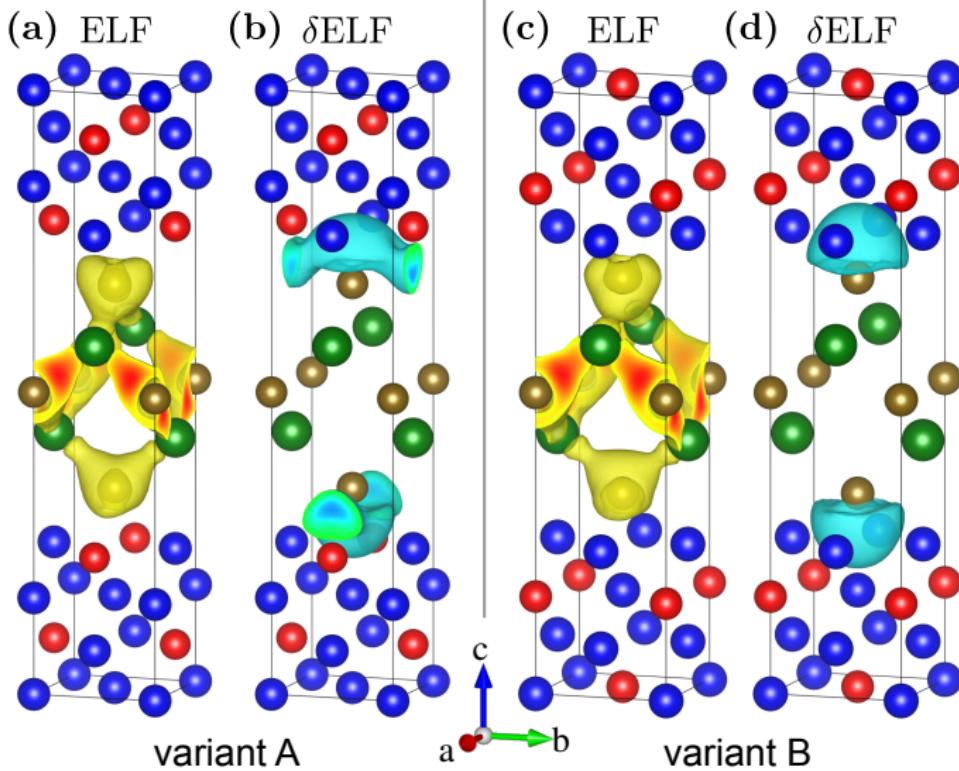
where $\tau_\sigma(\mathbf{r}) = \sum_i |\nabla \psi_{i\sigma}(\mathbf{r})|^2$, $\tau^w = |\nabla n|^2 / 8n$, which defines τ for a single orbital, and τ^u is the value for a uniform gas

$$\tau^u = \frac{3}{10} \left(\frac{3}{\pi^2} \right)^{\frac{2}{3}} n^{\frac{5}{3}}. \quad (3)$$

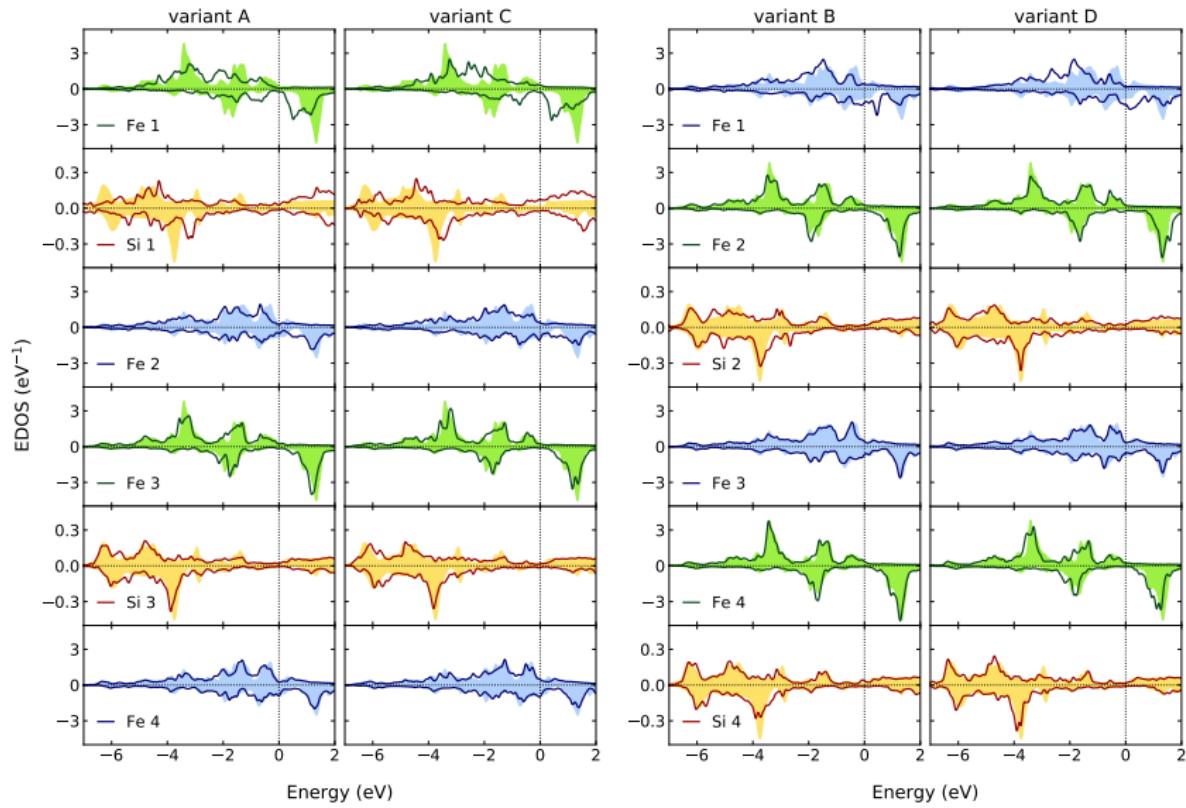
ELF is used to characterize the distribution of electron density

- ① slowly changing density, typical for metals, $\alpha \approx 1$, $\text{ELF} \approx \frac{1}{2}$.
- ② covalent bonds between two orbitals, $\alpha = 0$, $\text{ELF} = 1$.
- ③ weak noncovalent bonds between closed atomic shells, $\alpha \rightarrow \infty$, $\text{ELF} \rightarrow 0$.

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

$$P = \frac{N_{\uparrow}(E_F) - N_{\downarrow}(E_F)}{N_{\uparrow}(E_F) + N_{\downarrow}(E_F)}. \quad (4)$$

Magnetic anisotropy energy (MAE)

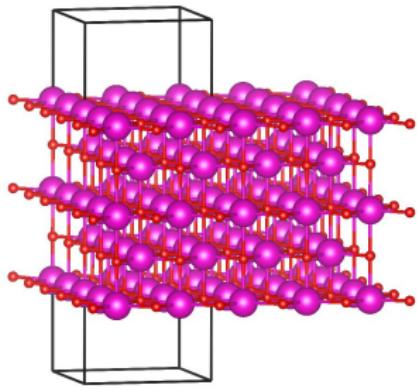
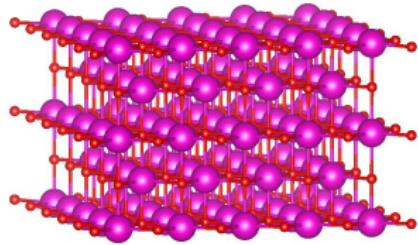
$$\Delta E = E[h_2 k_2 l_2] - E[h_1 k_1 l_1]. \quad (5)$$

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.

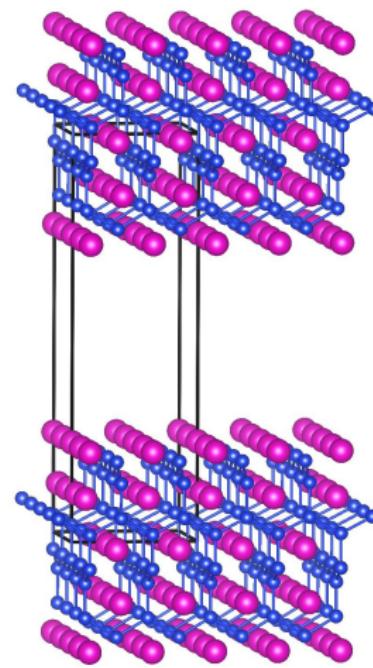
MAE (meV/p.u.c.)	Interface variants				Bulk Fe ₃ Si	
	A	B	C	D	Cubic	Tetragonal
$E_{[100]} - E_{[001]}$	0.10	0.17	0.10	-0.57	0.00	-0.26
$E_{[110]} - E_{[001]}$	-9.28	-7.38	-8.03	-1.25	0.01	-0.27
$E_{[110]} - E_{[100]}$	-9.38	-7.55	-8.13	-0.68	0.01	-0.01

Surfaces

$\text{EuO}(001)$

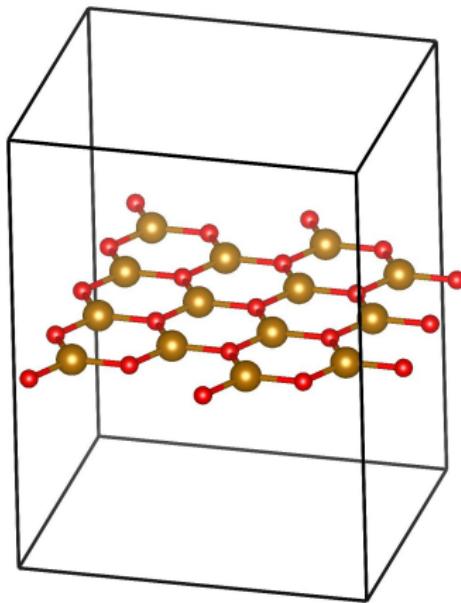


$\text{EuSi}_2(001)$

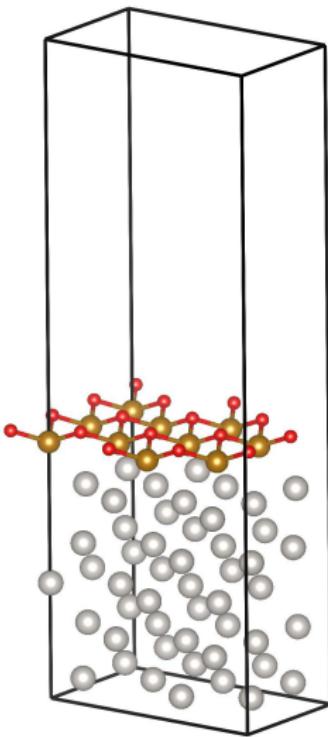


Monolayers and thin films

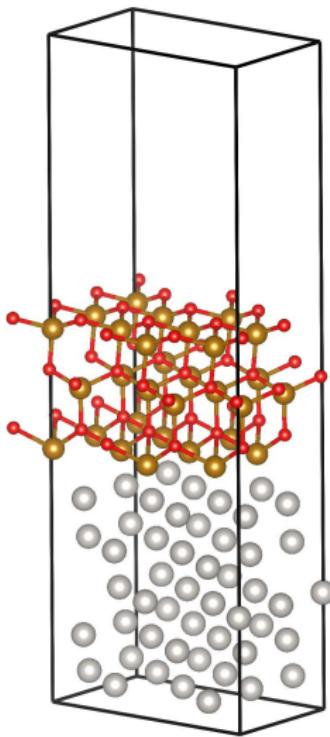
1ML FeO(111)



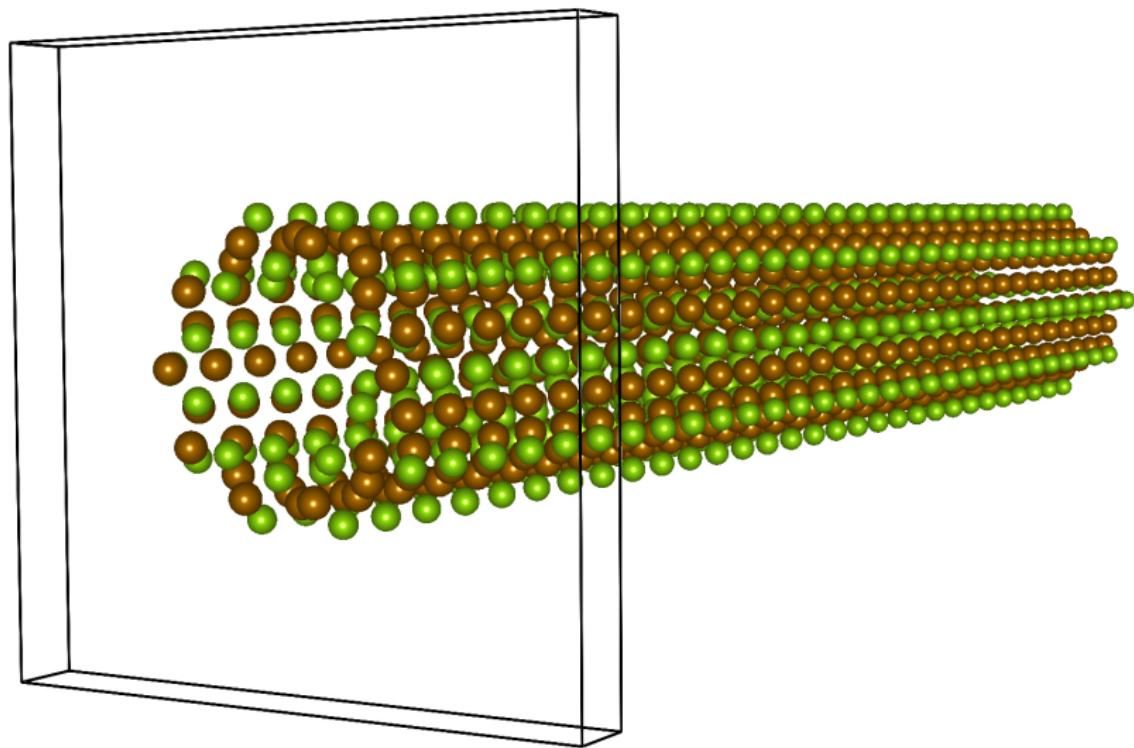
1ML FeO/Pt(111)



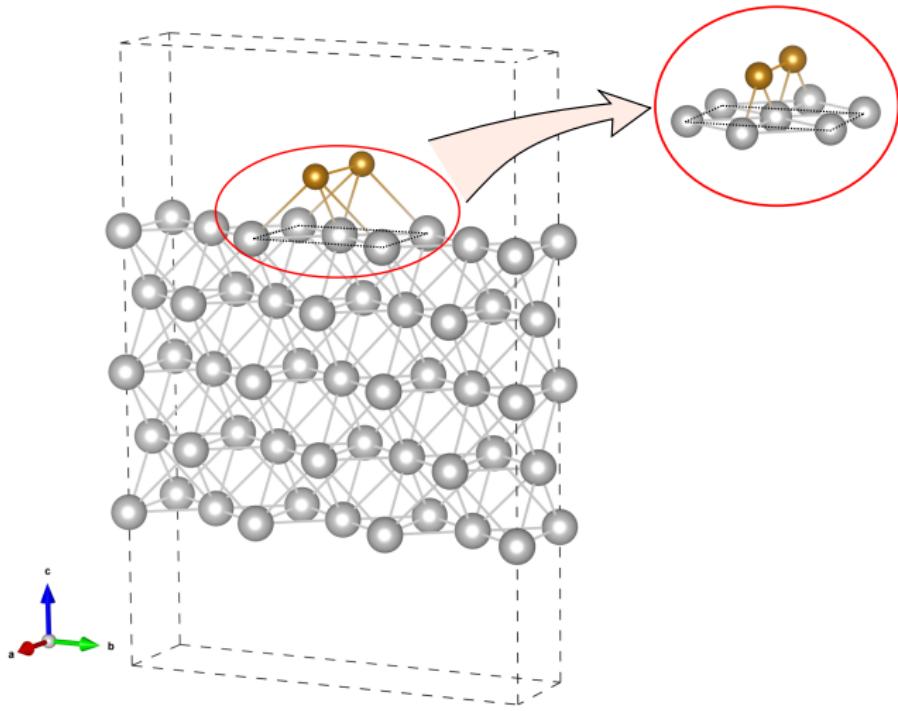
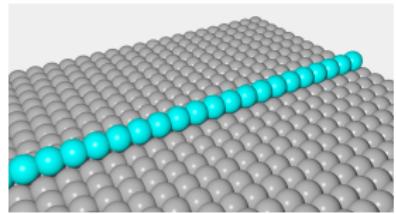
3ML FeO/Pt(111)



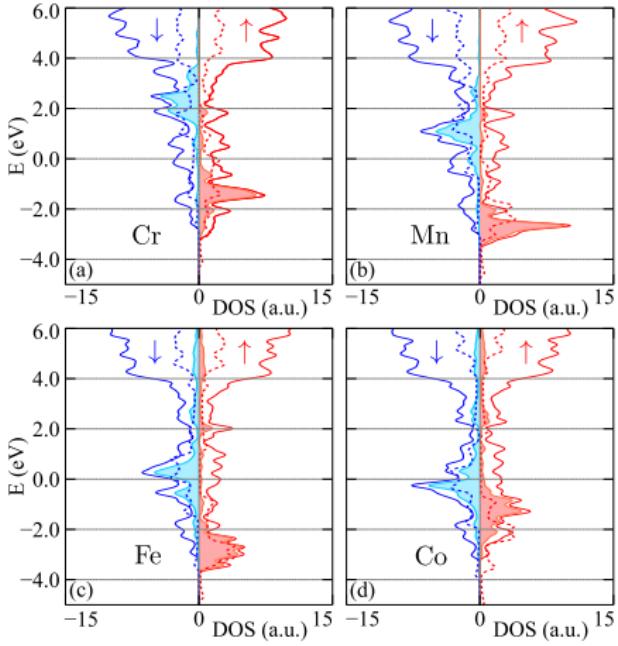
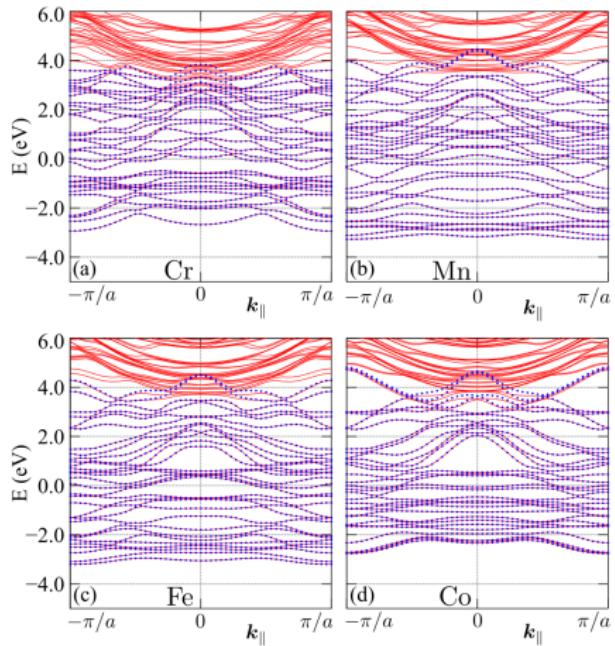
Nanotubes



Monoatomic chains

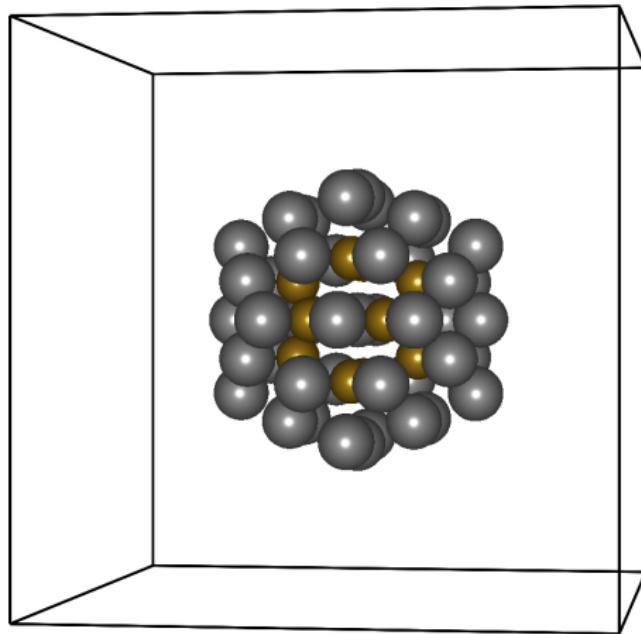


Monoatomic chains



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

Nanoparticles



Nanoparticles

