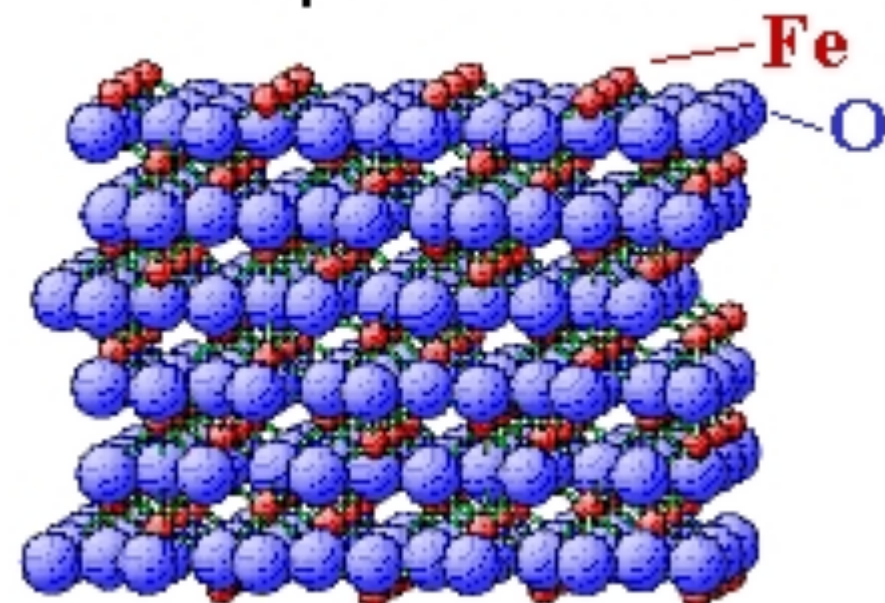


Stoichiometry, Structure, and Electronic Properties of Hematite (Fe_2O_3) (0001)

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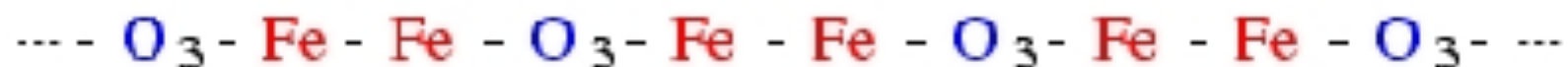
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Full-Potential-LAPW
calculations
with lattice relaxation
and magnetism
and STM experiments

Structures of Fe_2O_3 (0001) surface



Type of

surface:



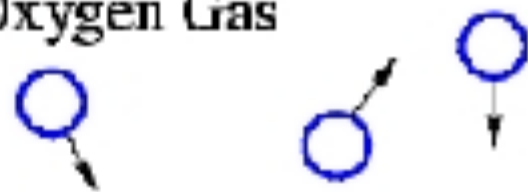
Surface



Bulk



Oxygen Gas



$$\mu_{\text{O}} < \mu_{\text{O}}(\text{gas})$$

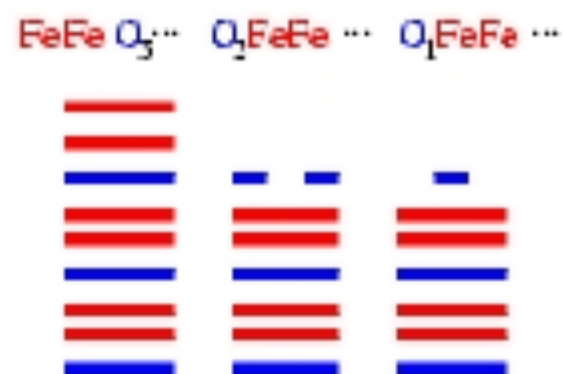
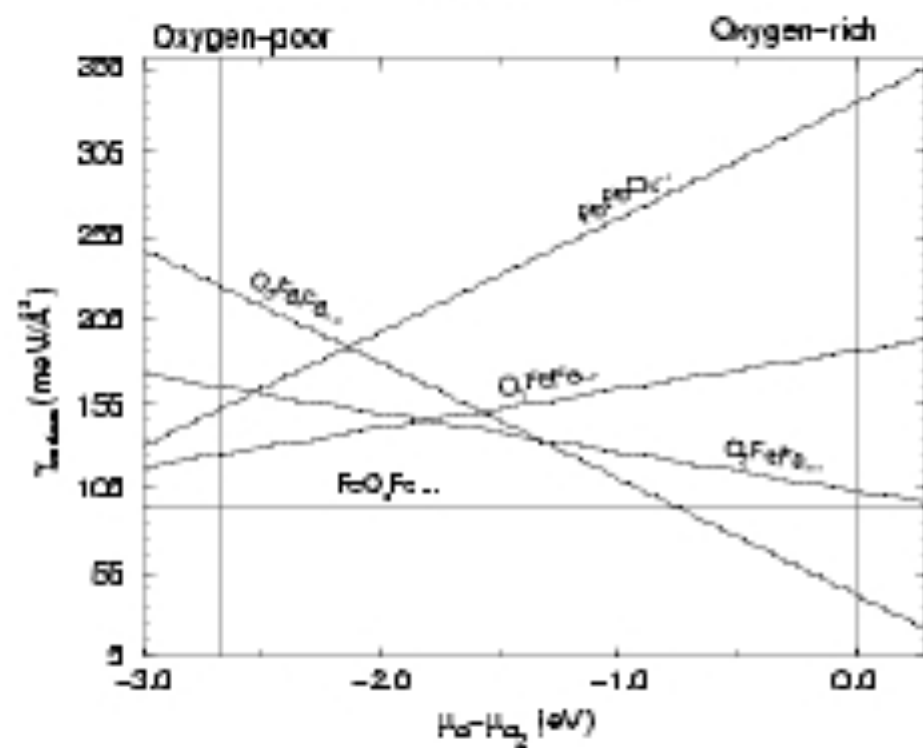
$$\mu_{\text{Fe}} < \mu_{\text{Fe}}(\text{bulk})$$

Surface

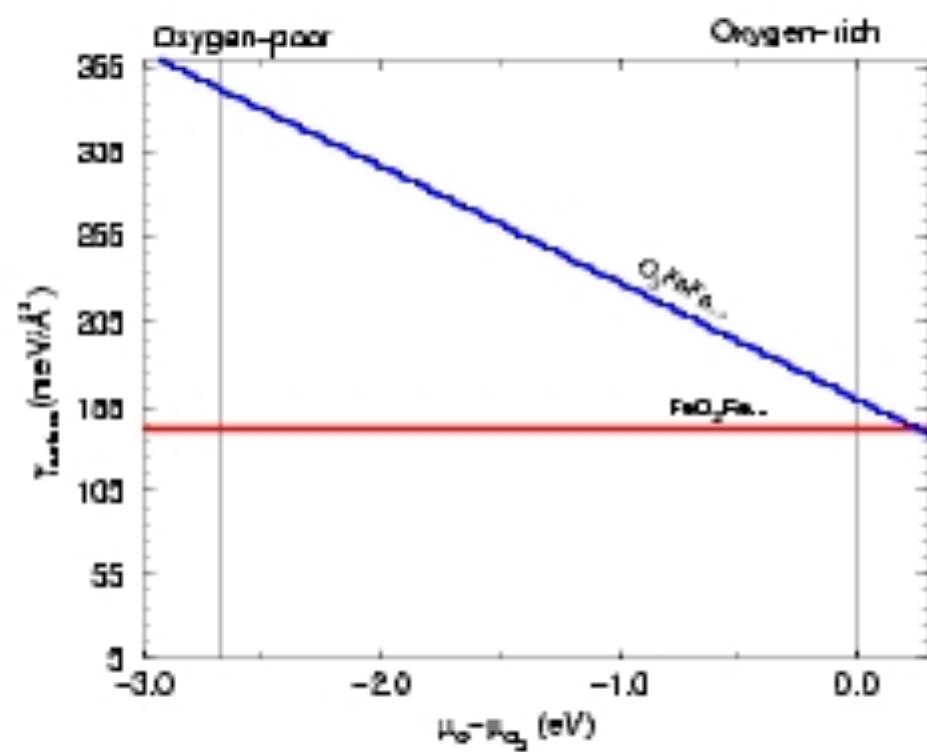
$$2\mu_{\text{Fe}} + 3\mu_{\text{O}} = \mu_{\text{Fe}_2\text{O}_3}$$

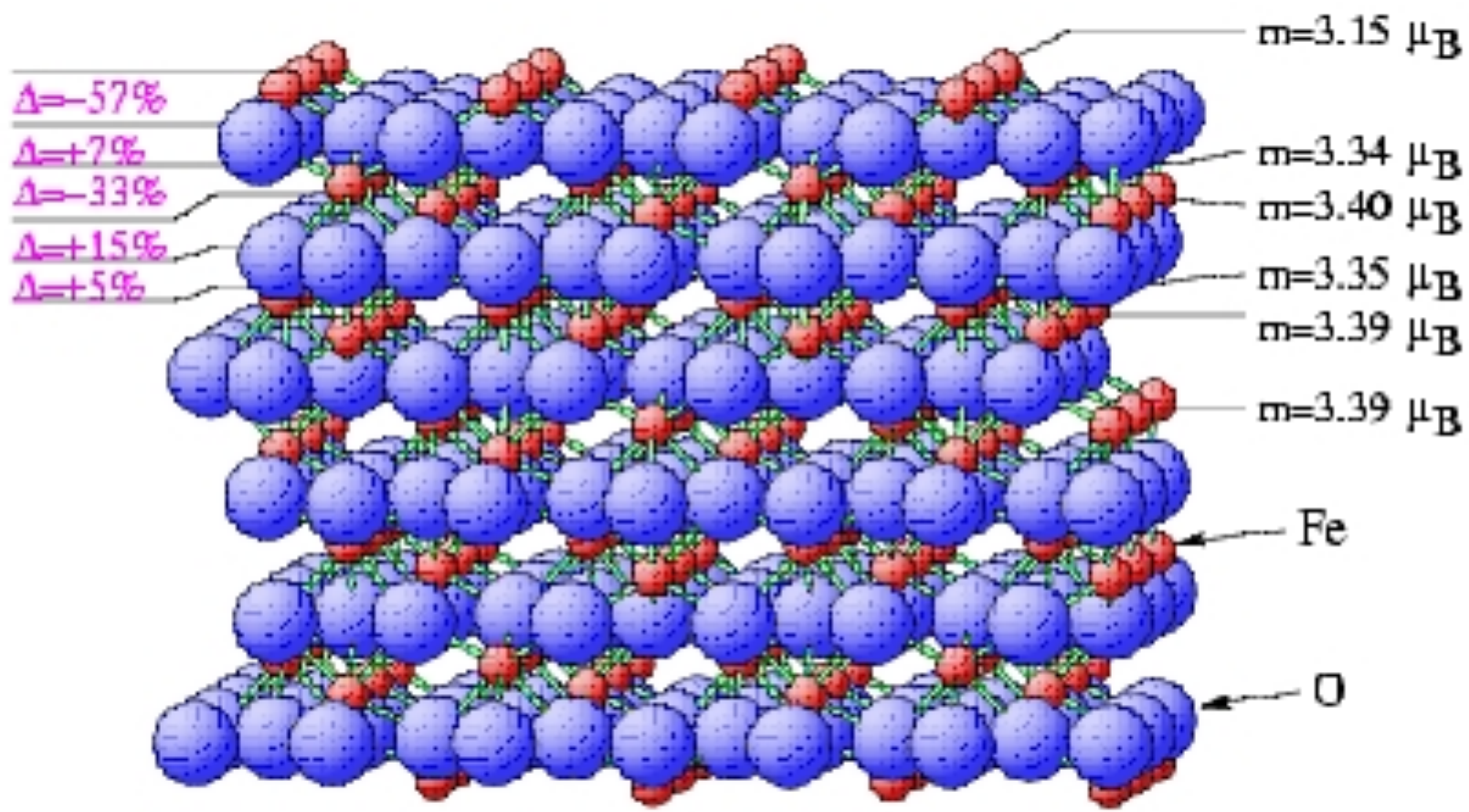
Fe_2O_3 Bulk

Relaxed Fe_2O_3 (0001) surfaces



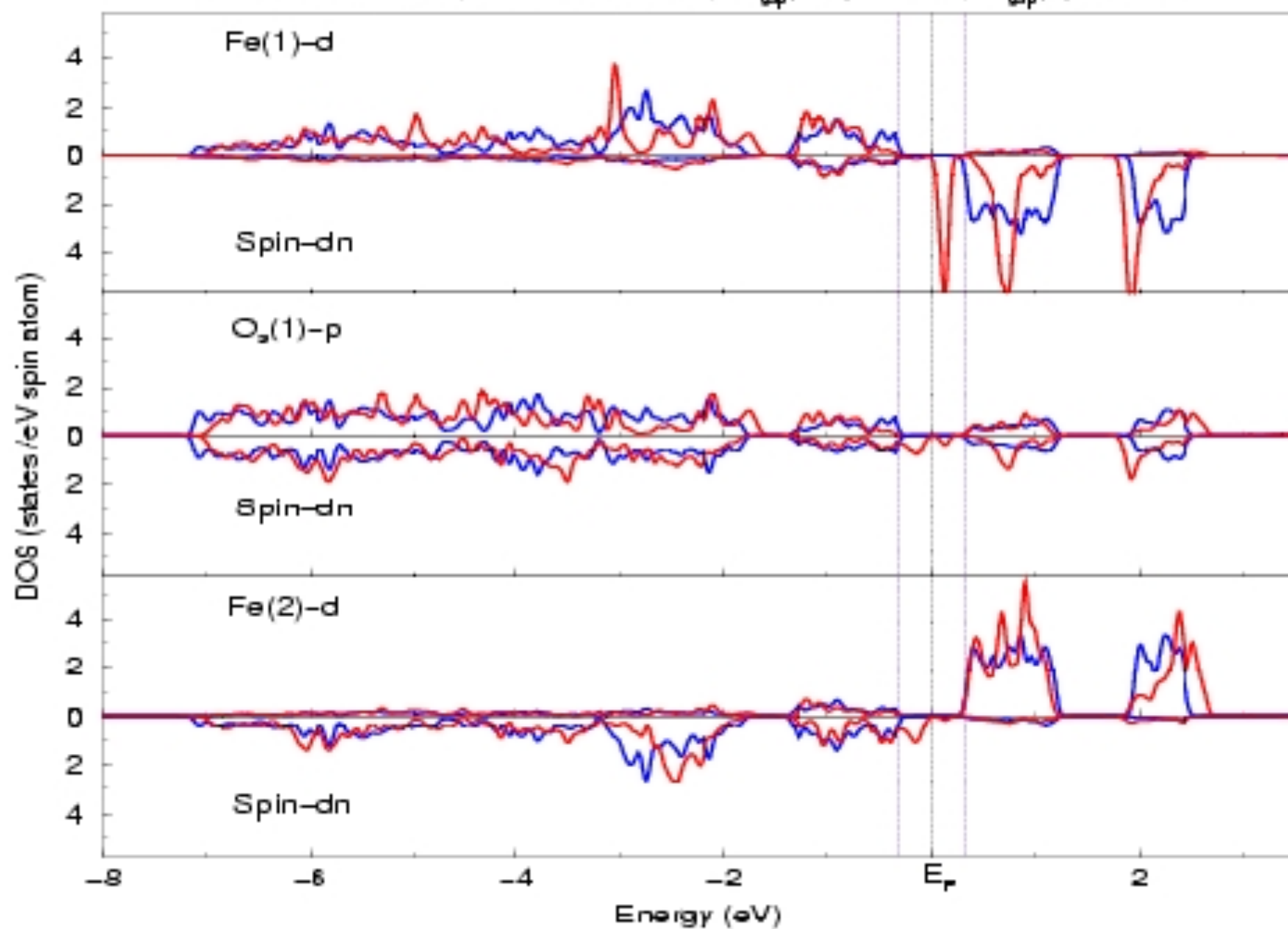
Un-relaxed Fe_2O_3 (0001) surfaces

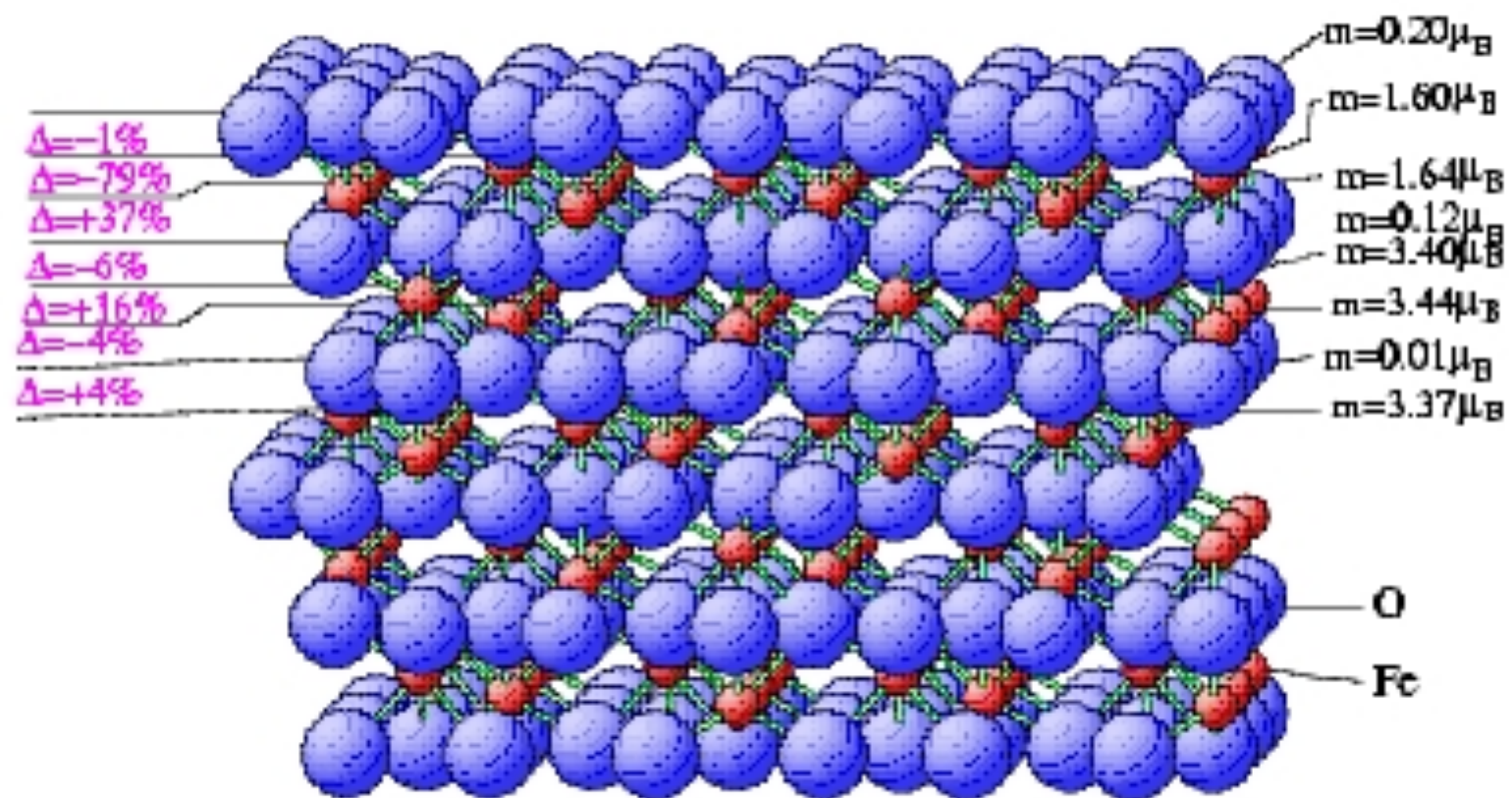




Partial DOS for Fe-terminated surface

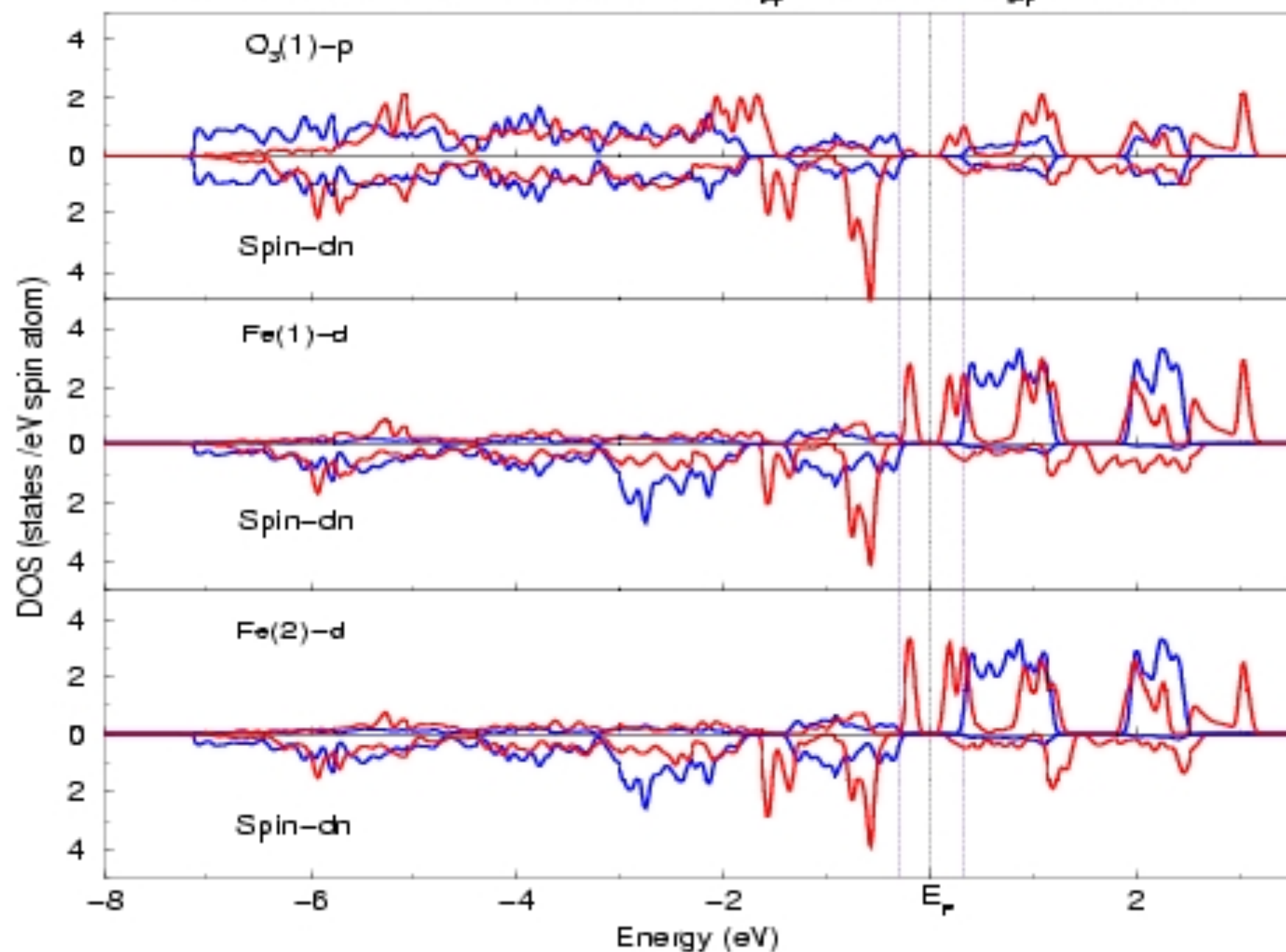
Gaussian width 0.03 eV, red color for surface; $\Delta E_{\text{gap}}(\text{bulk})=0.64$ eV, $\Delta E_{\text{gap}}(\text{S})=0.10$ eV

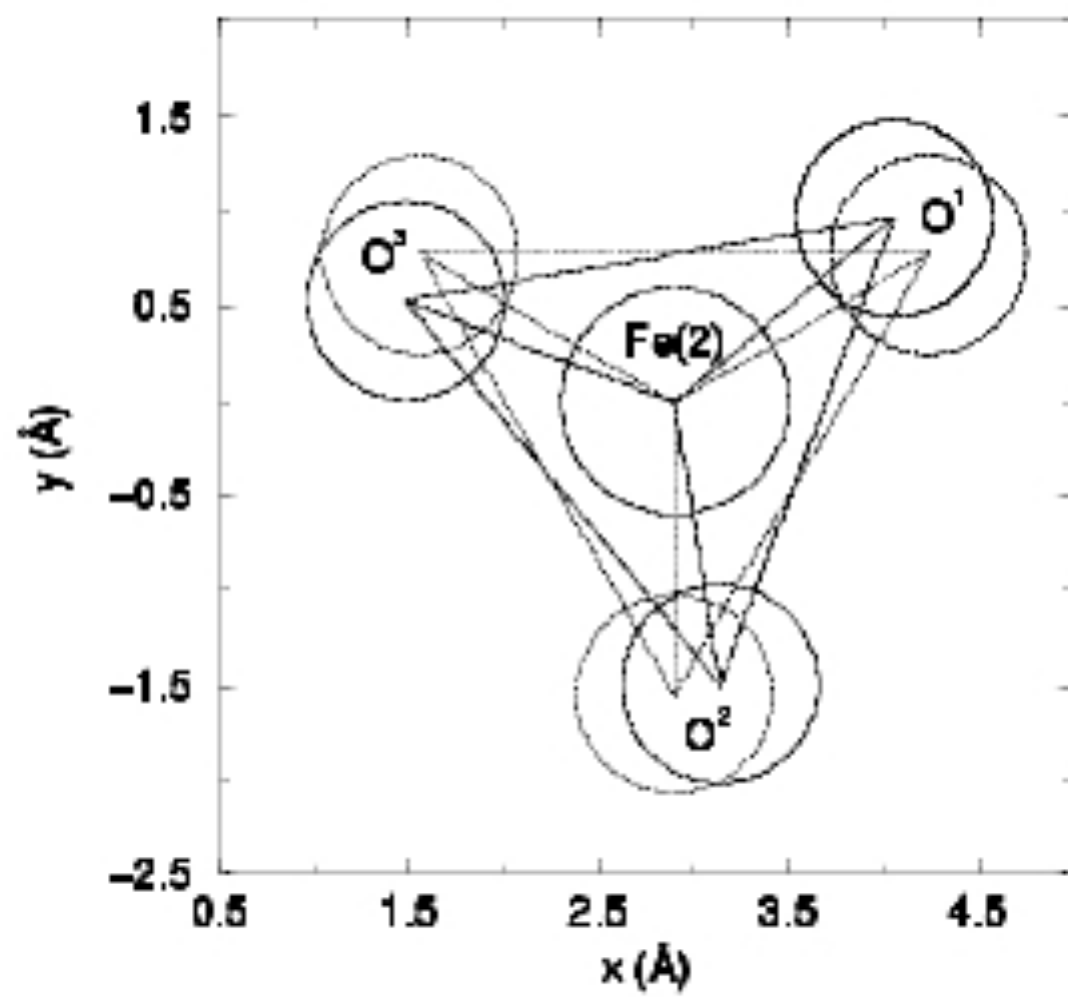


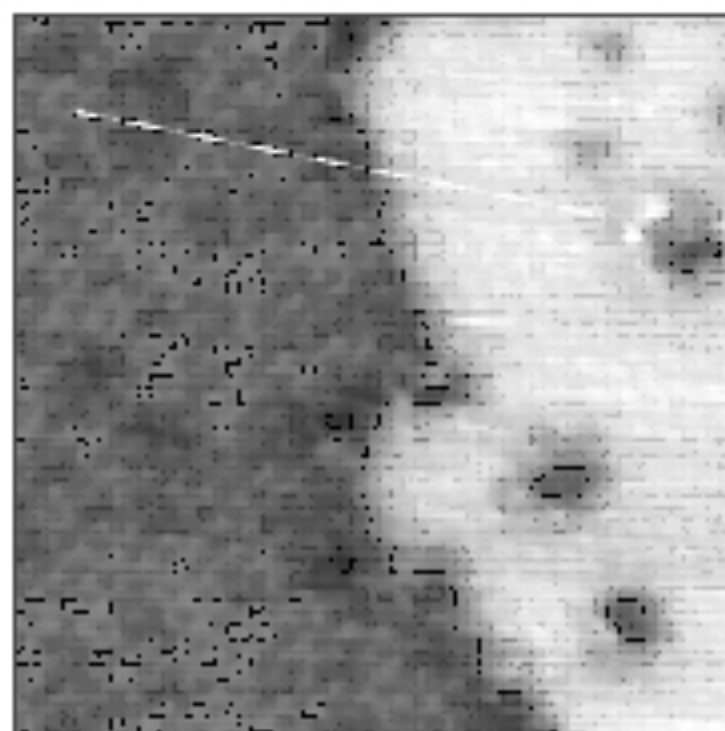


Partial DOS for O₃-terminated surface

Gaussian width 0.03 eV, red color for surface; $\Delta E_{\text{gap}}(\text{bulk})=0.64$ eV, $\Delta E_{\text{gap}}(\text{S})=0.23$ eV







Summary:

FP-LAPW calculations for Fe_2O_3 (0001) surface predict the existence of two domains with (1x1) periodicity: $\text{Fe-O}_3\text{-Fe-...}$ and $\text{O}_3\text{-Fe-Fe-...}$, as well as higher-energy metastable structures.

Lattice relaxations are huge (57 % for the Fe terminated, 79 % for the O_3 terminated surface).

Both surfaces exhibit surface states of Fe 3d character.

STM experiments at Fe_2O_3 films, created under high oxygen pressure conditions, confirm the presence of two domains.

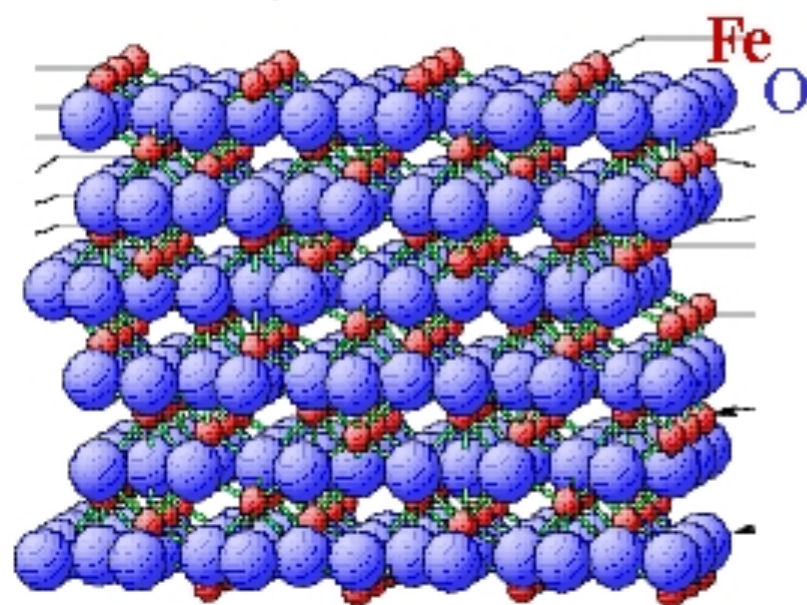
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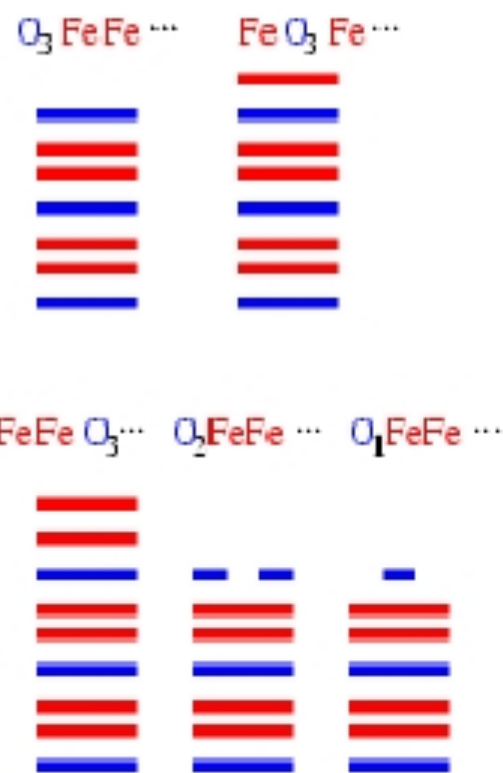
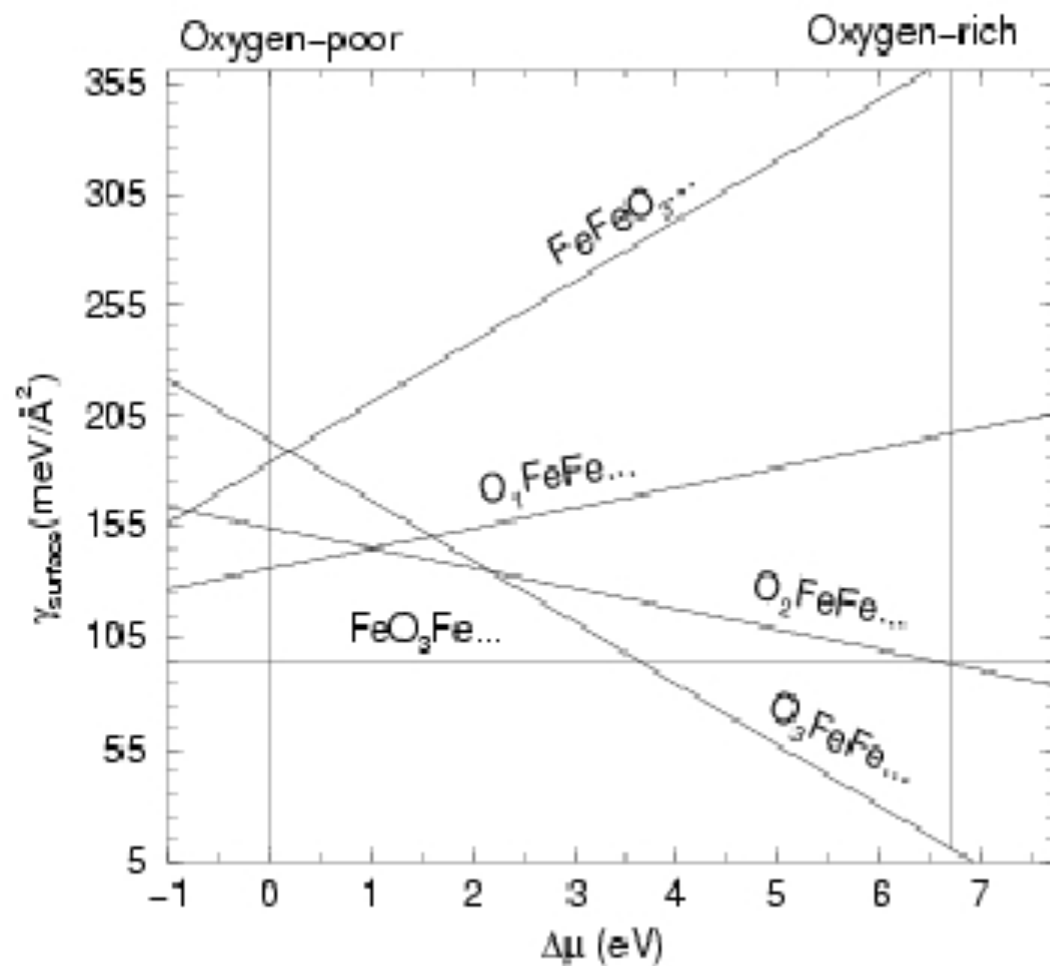
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