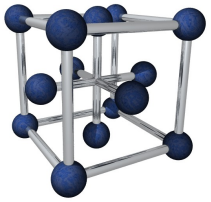
Gas adsorption on magnetic surfaces

David Gunn

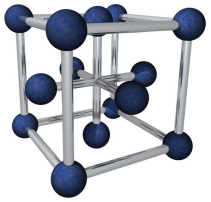
9th May 2007

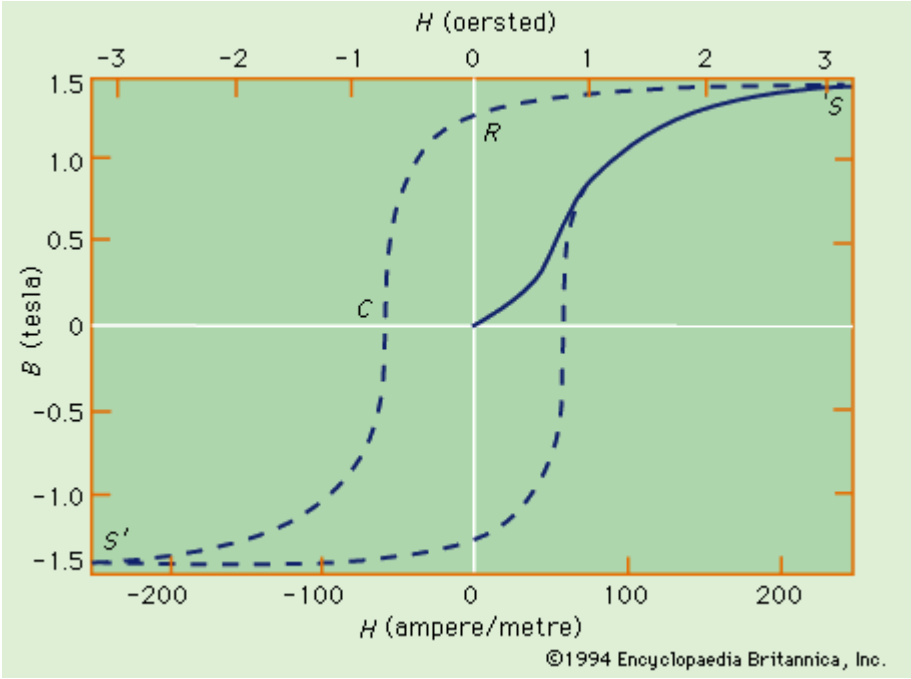
Contents



- Introduction
  - Magnetism and magnetic surfaces
  - Which surfaces, which adsorbates?
- Methodology
  - Calculation details
  - Choice of sites
- Results and Conclusions

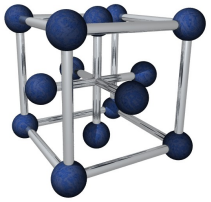
Magnetism and Surfaces





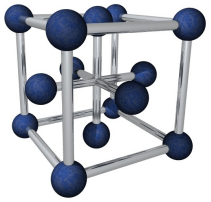
- Above Curie temperature the material becomes paramagnetic

Surface and Adsorbate choice



- Ferromagnetic elements: Fe, Co, Ni
- Simple atomic adsorbates: C, N, O
  - Produced experimentally through dissociation of CO, N_2 and O_2.
- *fcc* (110) surface

Surface and Adsorbate choice

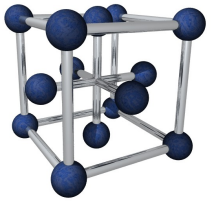


Reasons:

Detailed study of similar materials provides a comprehensive comparison

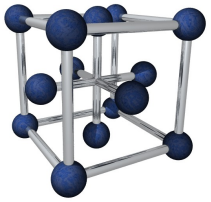
Analysis provides insight into nature of surface states and gas phase adsorption

Methodology

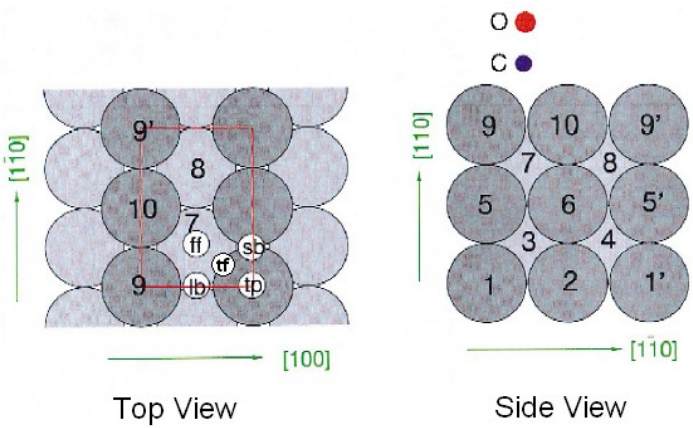


- CASTEP code
- Ultrasoft pseudopotentials
- Bader partitioning of electron density
- Slab calculation:
  - Four fixed layers simulating bulk, top two variable – adsorption only on top surface

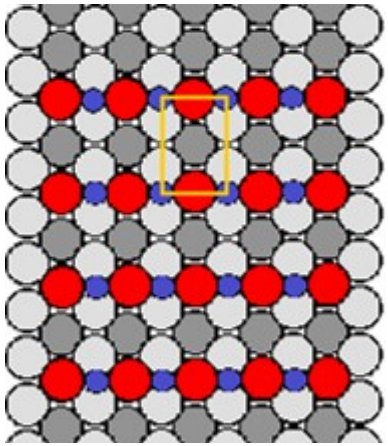
Choice of sites



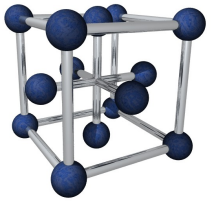
- 0.5ML and 1ML coverages of adsorbates in 5 sites:



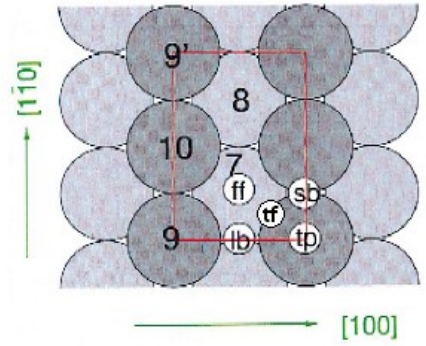
- Added row reconstruction:



Results - Oxygen

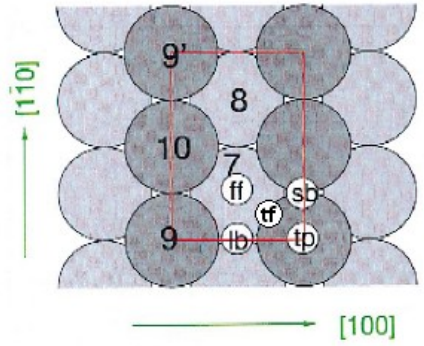


O	*Adsorbate*	
	½ ML	1 ML
Co	tfh	ffh
Ni	tfh	lb
Fe	tfh	ffh

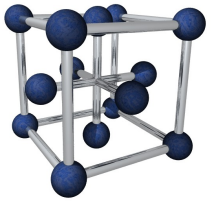


Results - Nitrogen

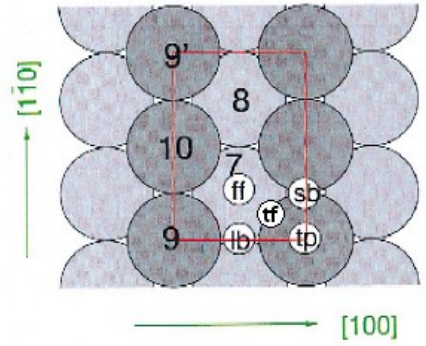
N	*Adsorbate*	
	½ ML	1 ML
Co	lb	lb
Ni	lb	lb
Fe	lb	lb



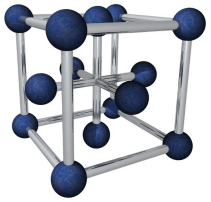
Results - Carbon



C	*Adsorbate*	
	½ ML	1 ML
Co	lb	tfh
Ni	lb	ffh
Fe	lb	lb

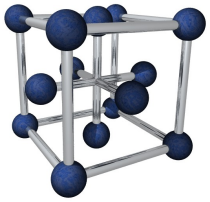


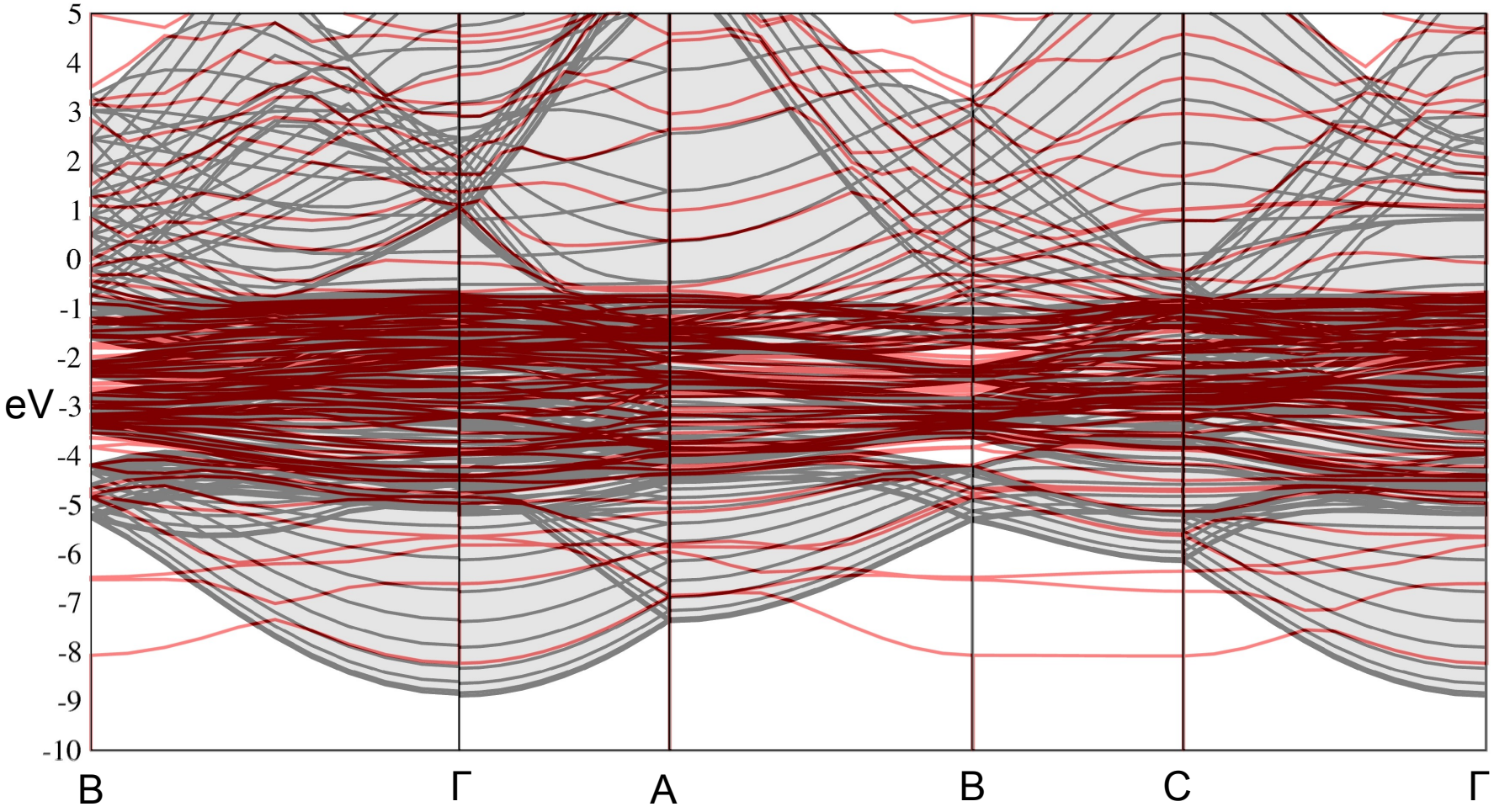
Results - Reconstruction



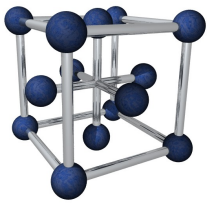
	O	N	C
Fe	X		
Co	X	X	
Ni	X	X	X

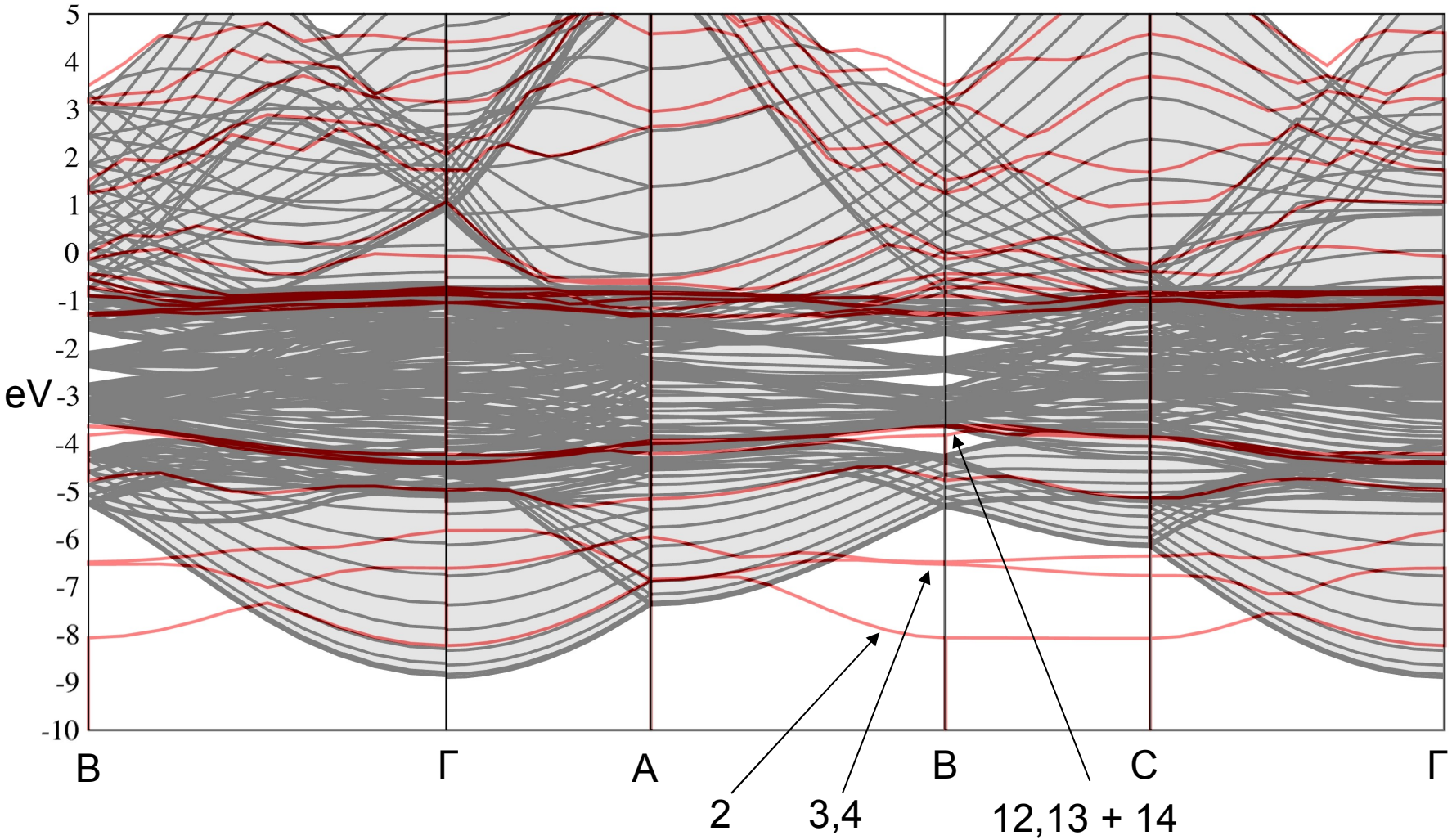
Results – OCo (recon)



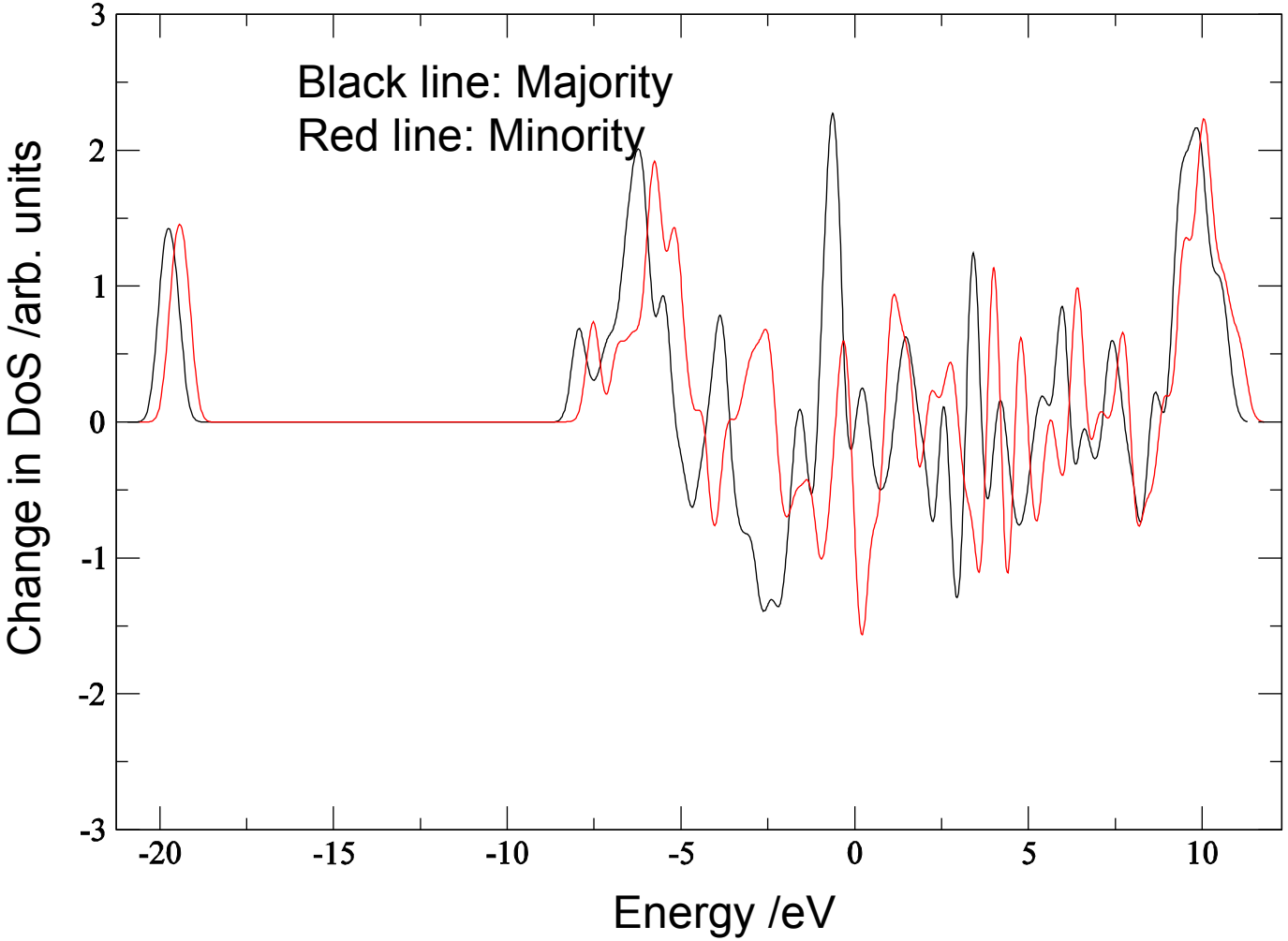


Results – OCo (recon)

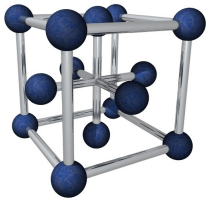




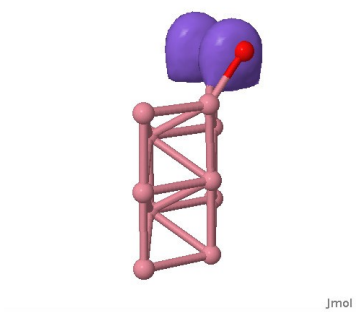
Results – OCo (recon)



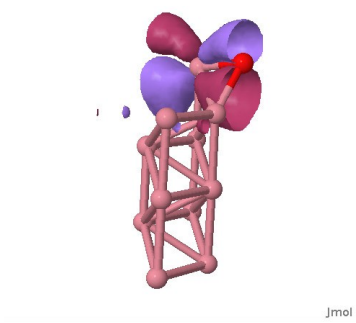
Results – OCo (recon)



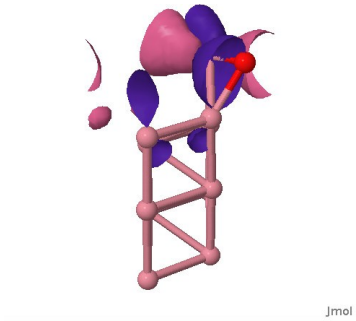
Band 2



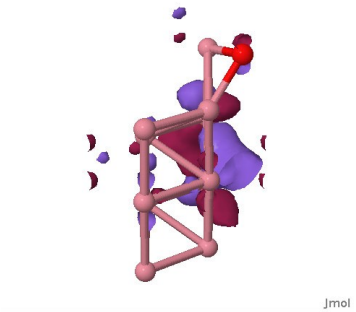
Band 3



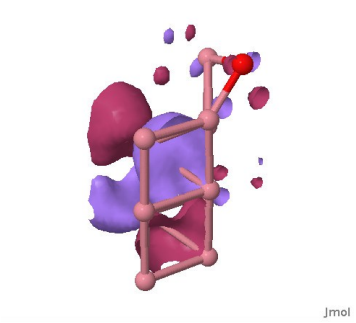
Band 4



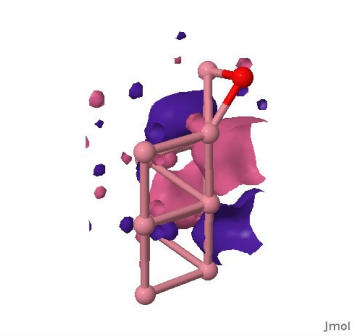
Band 12



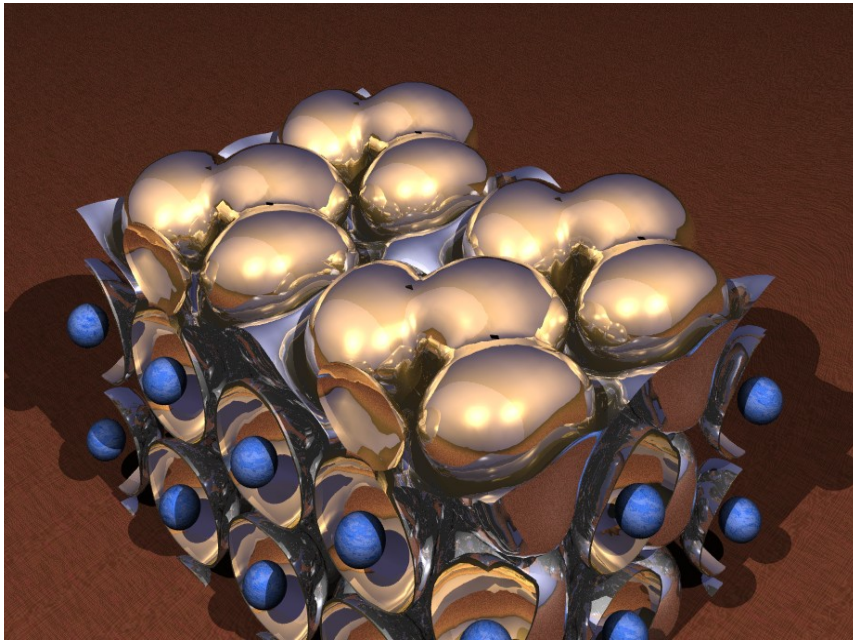
Band 13



Band 14



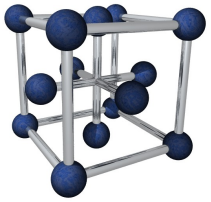
Results - OCo



- Isosurfaces of residual majority spin (gold) and minority spin (silver) for oxygen on Co(110)

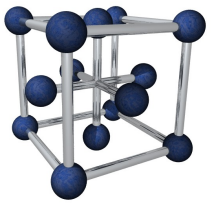
$$\left(\rho_{\alpha}-\rho_{\beta}\right)=\pm 3\times 10^{-3}\mu_{B}/\overset{o}{A}^{3}$$

Results – Fe (110) Spin moment



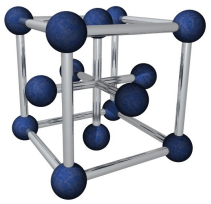
Layer	Clean	O		N		C	
		½ ML	1 ML	½ ML	1 ML	½ ML	1 ML
Adsorbate (average)		0.132	0.050	-0.088	-0.124	-0.196	-0.222
12	2.947	2.592	1.656	1.618	1.748	1.627	1.595
11	2.952	2.493	1.657	2.914	1.746	2.929	1.596
10	2.479	2.506	2.220	1.599	0.801	1.819	0.963
9	2.469	2.413	2.238	1.607	0.870	1.773	0.994
8	2.506	2.436	2.497	2.613	2.378	2.556	2.338
7	2.508	2.497	2.493	2.323	2.368	2.415	2.337
6	2.477	2.545	2.521	2.520	2.511	2.521	2.524
5	2.494	5.462	2.507	2.503	2.500	2.500	2.511

Results – Co (110) Spin moment



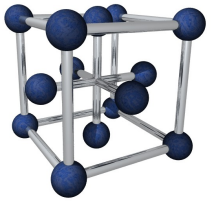
Layer	Clean	O		N		C	
		½ ML	1 ML	½ ML	1 ML	½ ML	1 ML
Adsorbate (average)		0.263	0.204	-0.018	-0.051	-0.145	-0.131
12	1.866	1.876	1.684	0.812	0.659	0.644	0.600
11	1.863	1.878	1.682	2.015	0.663	2.033	0.600
10	1.636	1.799	1.653	1.505	1.130	1.628	0.820
9	1.626	1.707	1.644	1.495	1.094	1.286	0.833
8	1.694	1.678	1.687	1.762	1.754	1.738	1.673
7	1.697	1.673	1.692	1.631	1.753	1.600	1.672
6	1.688	1.705	1.659	1.670	1.641	1.670	1.661
5	1.678	1.660	1.643	1.659	1.628	1.653	1.645

Results – Ni (110) Spin moment



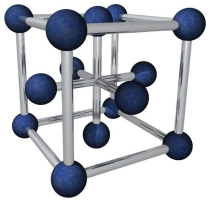
Layer	Clean	O		N		C	
		½ ML	1 ML	½ ML	1 ML	½ ML	1 ML
Adsorbate (average)		0.208	0.204	0.001	-0.004	-0.014	0.001
12	0.740	0.666	0.380	-0.019	-0.012	0.032	0.074
11	0.740	0.668	0.387	0.672	-0.012	0.664	0.040
10	0.621	0.657	0.675	0.344	0.101	0.243	0.414
9	0.609	0.605	0.651	0.329	0.092	0.226	0.391
8	0.614	0.614	0.651	0.612	0.552	0.588	0.614
7	0.616	0.612	0.651	0.612	0.552	0.527	0.600
6	0.622	0.638	0.607	0.607	0.587	0.606	0.603
5	0.614	0.608	0.599	0.606	0.583	0.598	0.590

Results – Reconstruction (Fe)



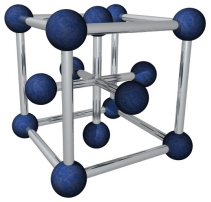
Layer	Clean	O	N	C
		½ ML	½ ML	½ ML
Adsorbate (average)		0.179		
11	2.952	2.648		
10	2.479	2.672		
9	2.469	2.691		
8	2.506	2.535		
7	2.508	2.504		
6	2.477	2.511		
5	2.494	2.495		

Results – Reconstruction (Co)



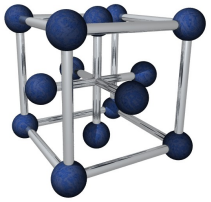
Layer	Clean	O	N	C
		½ ML	½ ML	½ ML
Adsorbate (average)		0.198	-0.007	
11	1.863	1.637	0.814	
10	1.636	1.785	1.604	
9	1.626	1.785	1.599	
8	1.694	1.728	1.759	
7	1.697	1.668	1.645	
6	1.688	1.650	1.666	
5	1.678	1.635	1.651	

Results – Reconstruction (Ni)



Layer	Clean	O	N	C
		½ ML	½ ML	½ ML
Adsorbate (average)		0.167	0.035	-0.025
11	0.740	0.578	0.029	0.015
10	0.621	0.705	0.375	0.142
9	0.609	0.707	0.371	0.151
8	0.614	0.681	0.641	0.593
7	0.616	0.609	0.578	0.457
6	0.622	0.625	0.615	0.608
5	0.614	0.613	0.605	0.601

Conclusions



- General trend identified concerning bonding nature of C, N and O on magnetic surfaces.
- Detailed look at electronic structure reveals complex picture:
  - No states strongly localised on adsorbate identified near the Fermi level (so far)
  - p-states heavily delocalised over a large energy generally speaking

Acknowledgements

- Steve Jenkins
- The Surface Science Group
- EPSRC