Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information:

Electronic and structural properties of arsenopyrite bulk and its cleavage surfaces – A DFT study.

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Table S1: Surfaces correspondence in $C2_1/d$ and $P2_1/c$ unit cells.

$C2_1/d$	$P2_1/c$
110	100
100	101
001	010
1-10	001
101	121
111	110
010	10-1

Table S2: Critical points in QTAIM analysis.

Critical points	$\rho(r_c)$ *	$\nabla^2\rho(r_c)$ *	Chemical meaning
Fe	6.2235	-73.0292	
As	0.5412	-18.0058	
S	0.3588	-10.8180	
b1	0.0721	0.0492	Fe-As
b2	0.0961	0.1501	Fe-S
b3	0.0733	0.0730	Fe-As
b4	0.0924	0.1996	Fe-S
b5	0.0725	0.0475	Fe-As
b6	0.0828	-0.0075	As-S
b7	0.0881	0.2232	Fe-S
r1	0.0326	0.0546	Fe…Fe long
r2	0.0430	0.0539	Fe…Fe short
r3	0.0145	0.0427	
r4	0.0109	0.0297	
r5	0.0145	0.0379	
r6	0.0151	0.0443	
r7	0.0174	0.0417	
r8	0.0162	0.0431	
r9	0.0078	0.0192	
c1	0.0119	0.0398	
c2	0.0081	0.0274	
c3	0.0101	0.0302	
c4	0.0078	0.0232	
c5	0.0078	0.0228	

* In atomic units.

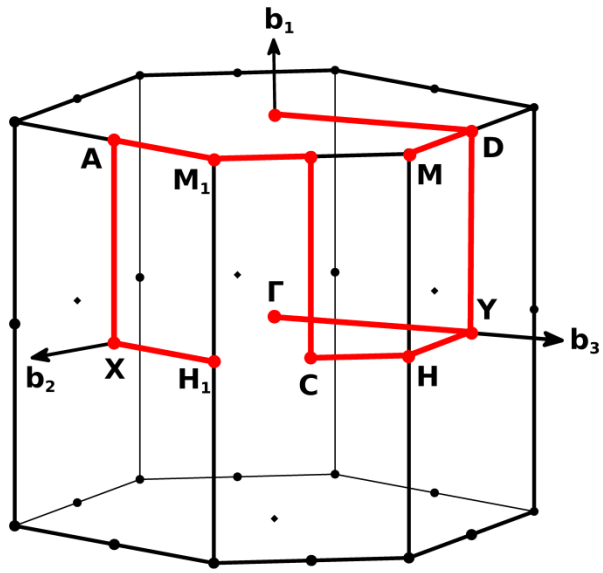
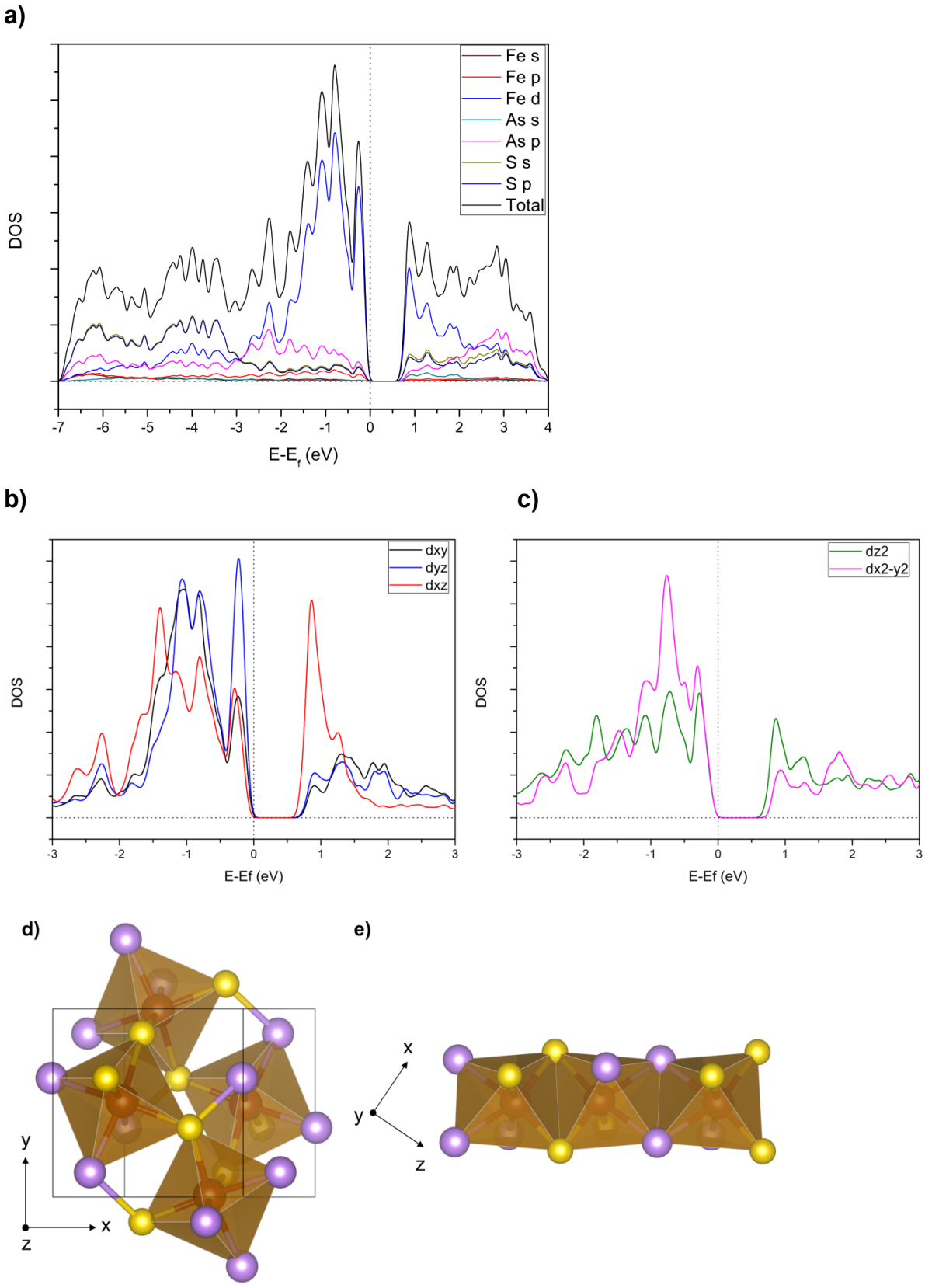


Figure S1: **K** points path for band structure calculation.



Figures S2: a) DOS projected over the atomic orbitals of arsenopyrite; b) and c) DOS projected over iron *d* orbitals plotted using a Gaussian width of 0.005 Ry; d) and e) orbitals orientation.

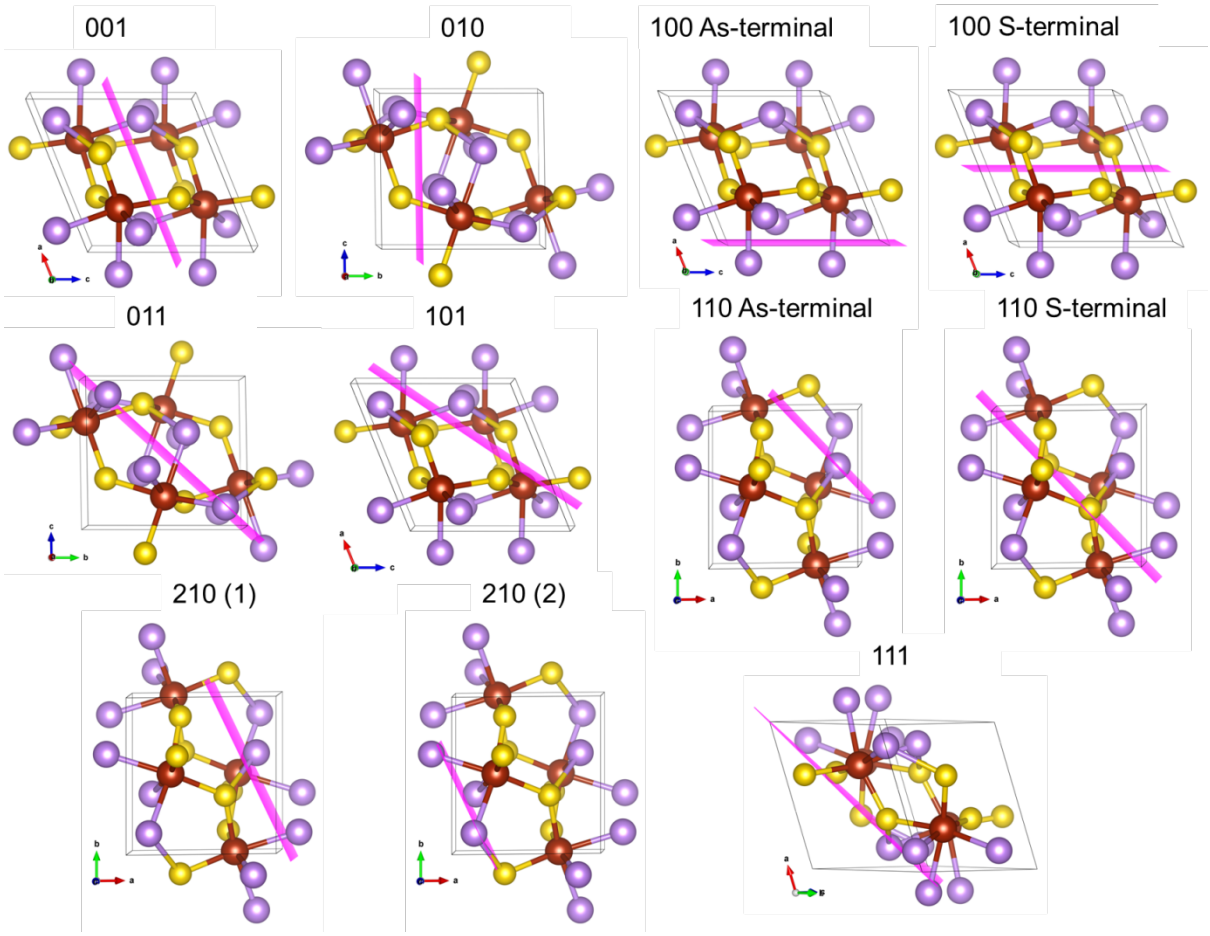


Figure S3: Arsenopyrite cleavage planes. Iron is in red, sulfur in yellow and arsenic in purple. Miller indices are based on the $P2_1/c$ symmetry.

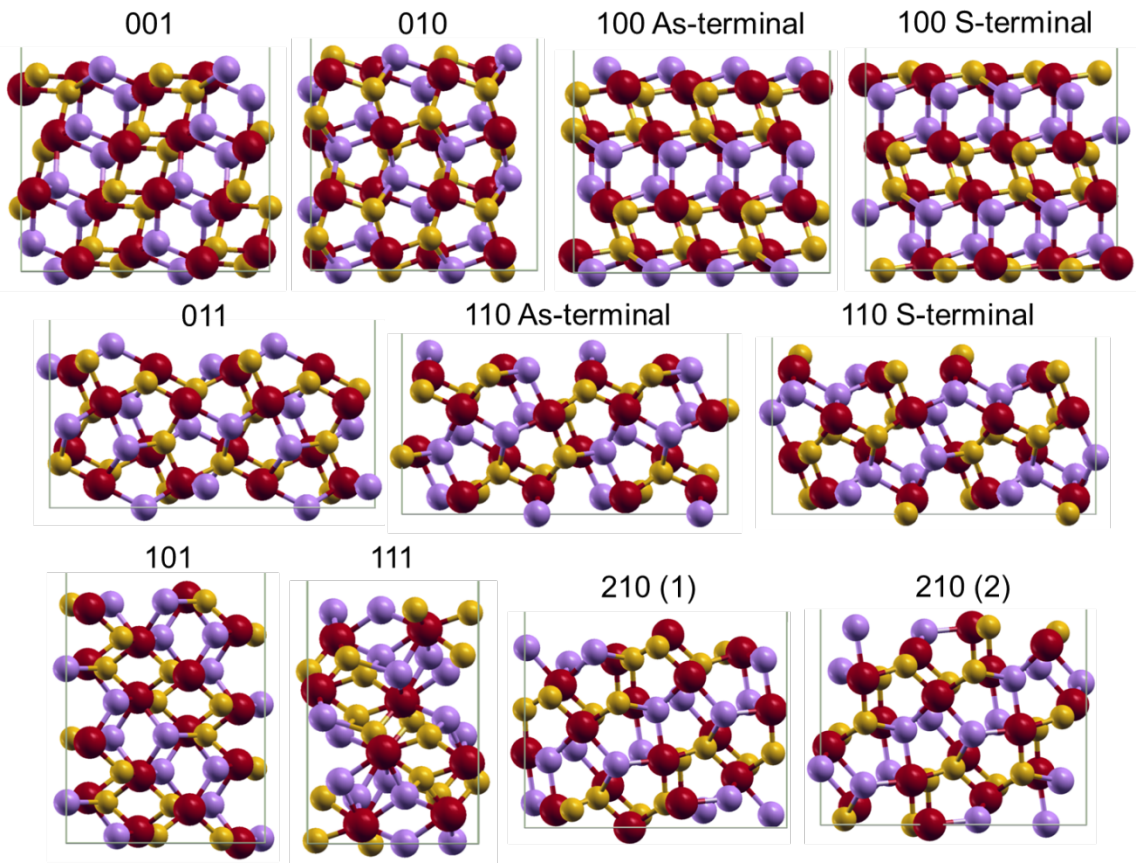


Figure S4: Arsenopyrite cleavage surfaces used to perform the calculations. Iron is in red, sulfur in yellow and arsenic in purple. Miller indices are based on the **$P2_1/c$** symmetry.