Possibility of p-type and n-type doping in bulk FeS_2

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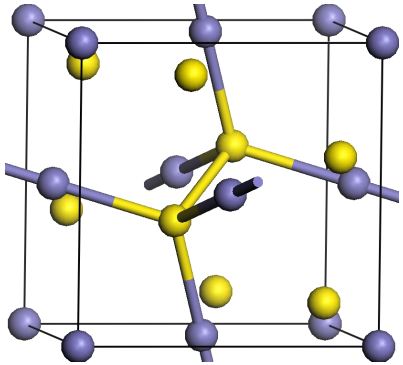
I. Background



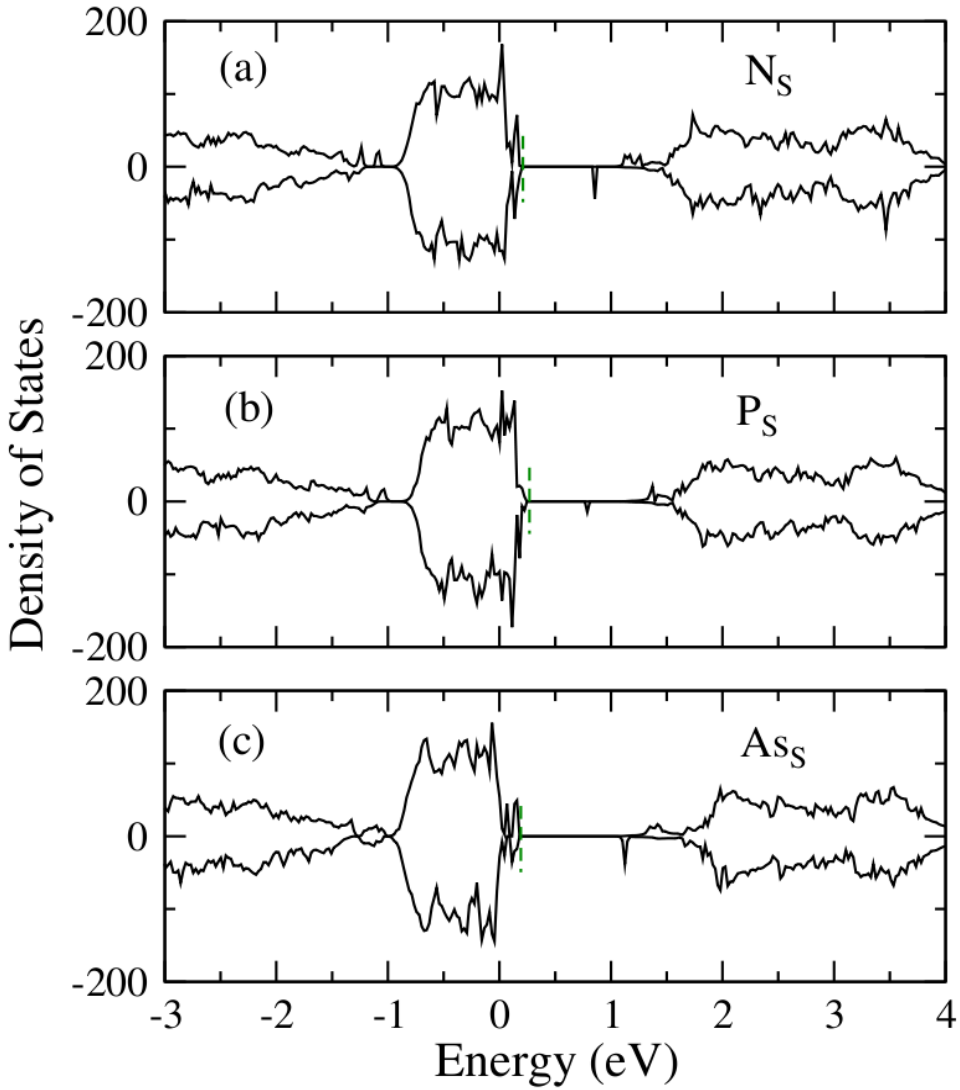
Experimental studies on doping in FeS_2 have lasted over twenty years.

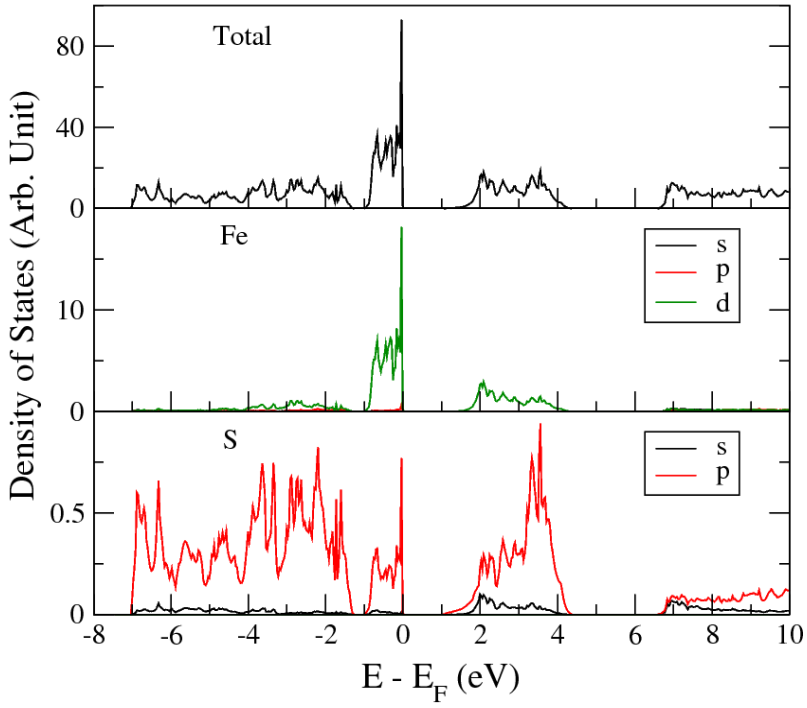
Metal dopants are all donors, while P and As seem to be acceptor, but the results of p-type are inconclusive.

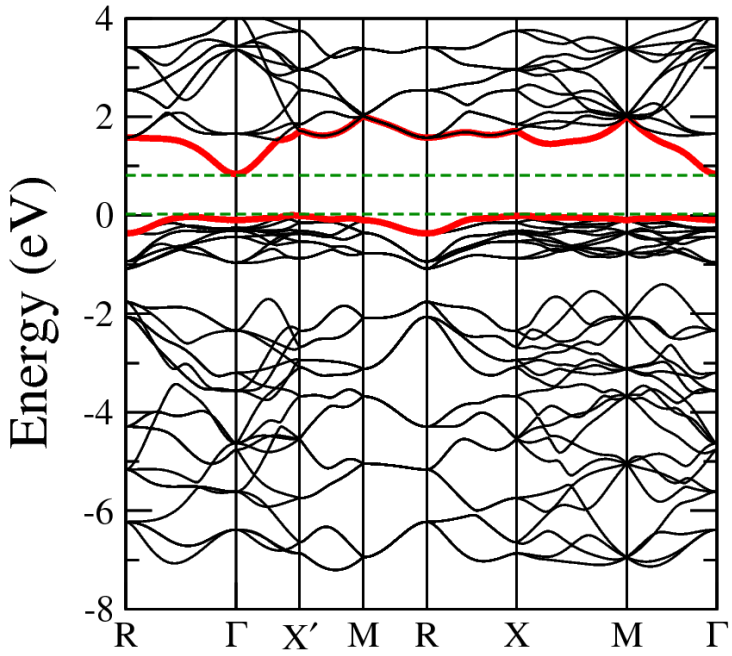
1	1 H																2 He
2	3 Li	4 Be											5 B	6 C	7 N	8 O	9 F	10 Ne
3	11 Na	12 Mg											13 Al	14 Si	15 P	16 S	17 Cl	18 Ar
4	19 K	20 Ca	21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr
5	37 Rb	38 Sr	39 Y	40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe
6	55 Cs	56 Ba	* 71 Lu	72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	79 Au	80 Hg	81 Tl	82 Pb	83 Bi	84 Po	85 At	86 Rn
7	87 Fr	88 Ra	** 103 Lr	104 Rf	105 Db	106 Sg	107 Bh	108 Hs	109 Mt	110 Ds	111 Rg	112 Cn	113 Uut	114 Uuq	115 Uup	116 Uuh	117 Uus	118 Uuo

II. Results: p-type and n-type doping

Doping with N, P, or As

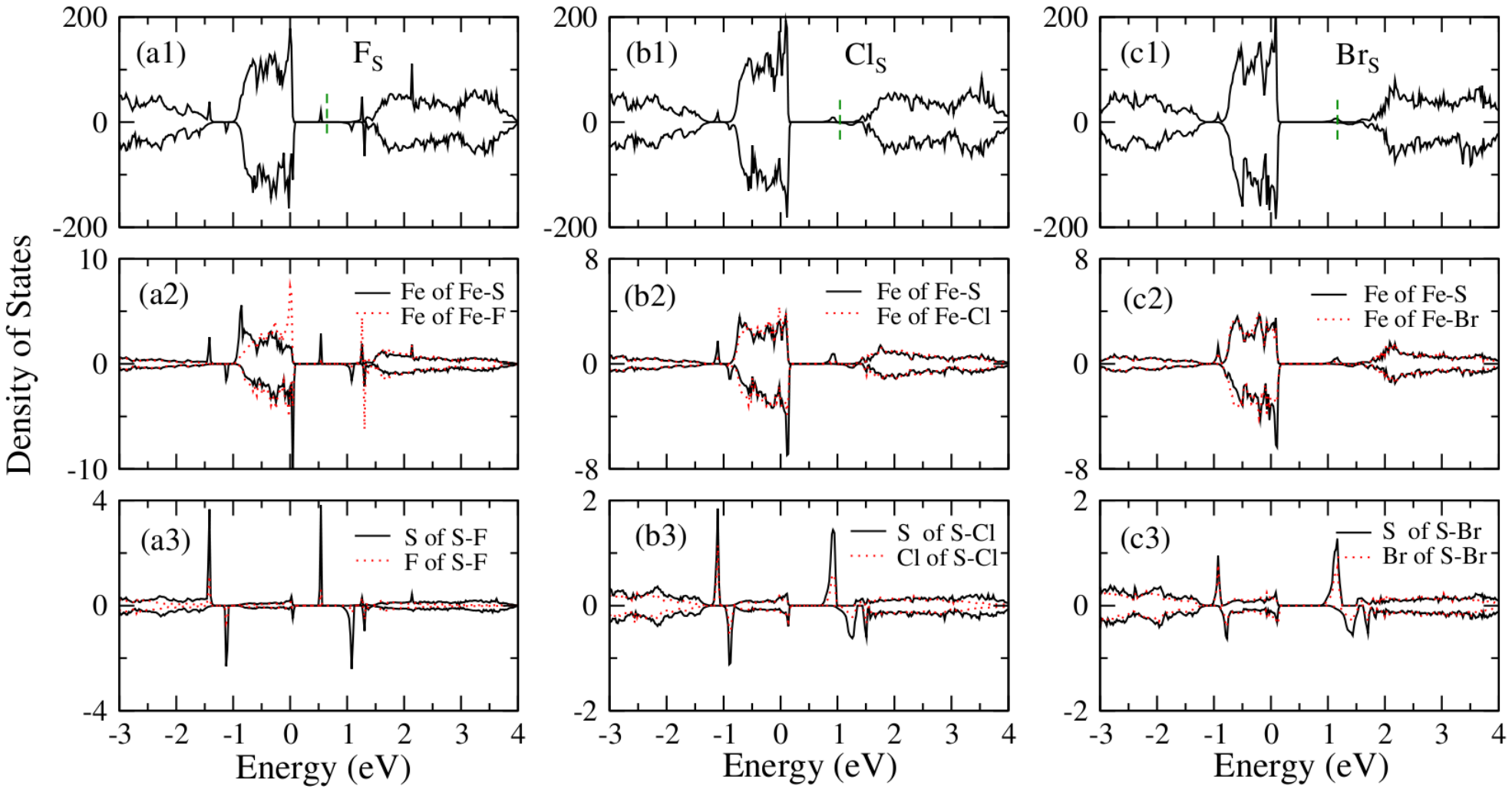






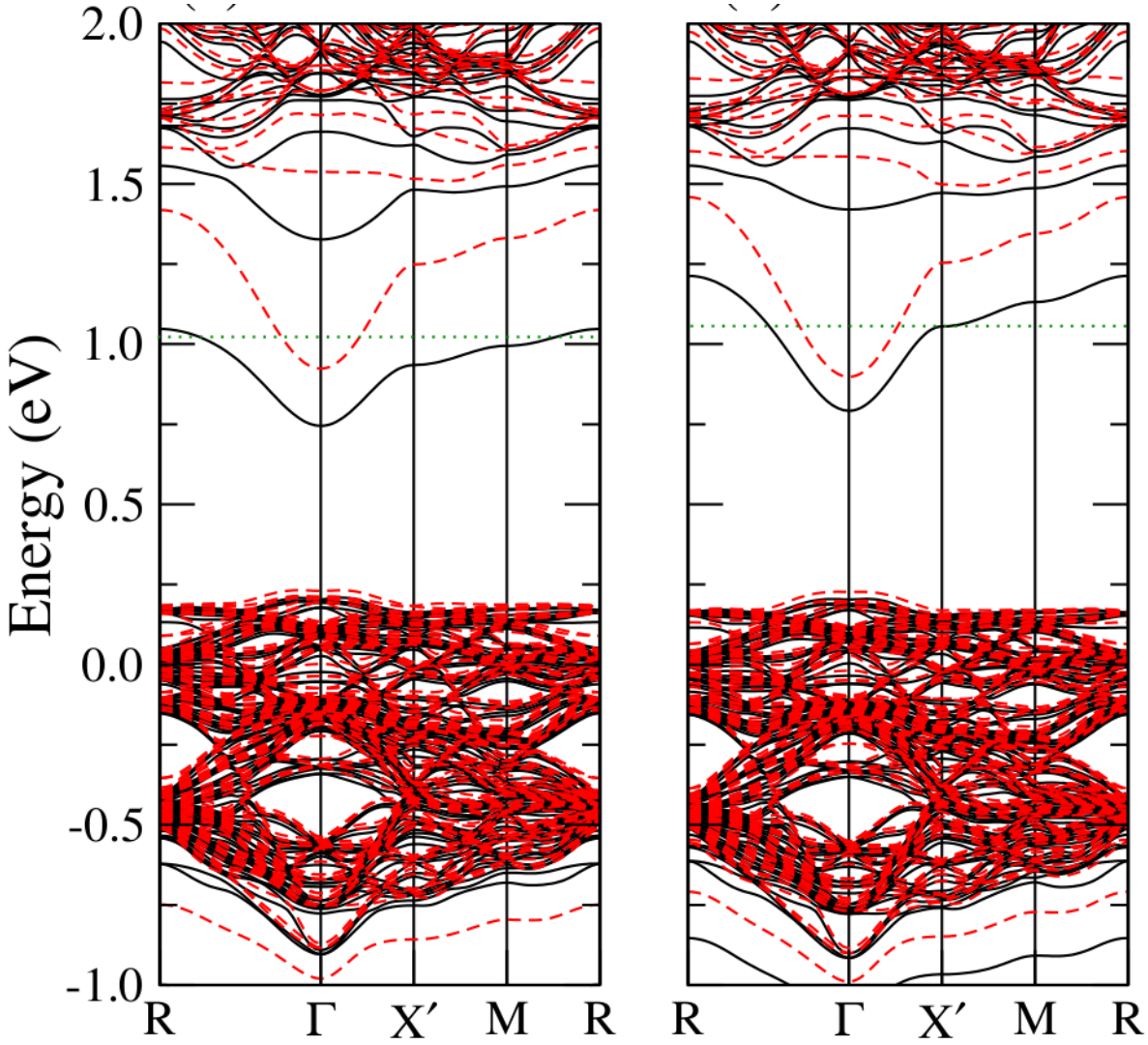
II. Results: p-type and n-type doping

Doping with F, Cl or Br



II. Results: p-type and n-type doping

Band structures of Cl- or Br-doped FeS_2

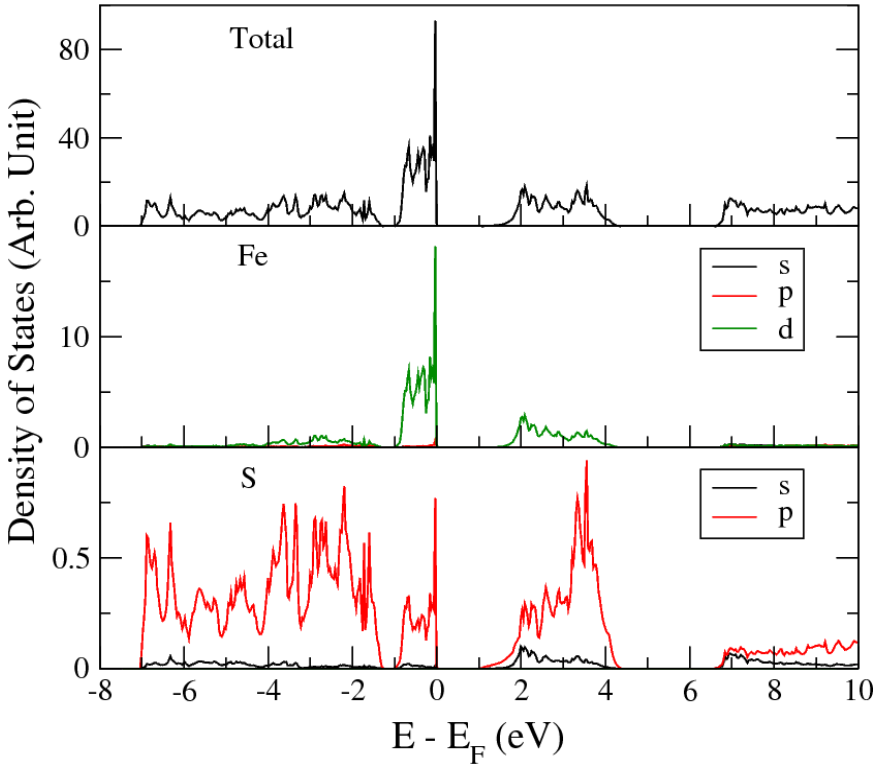


Cl-doped Br-doped

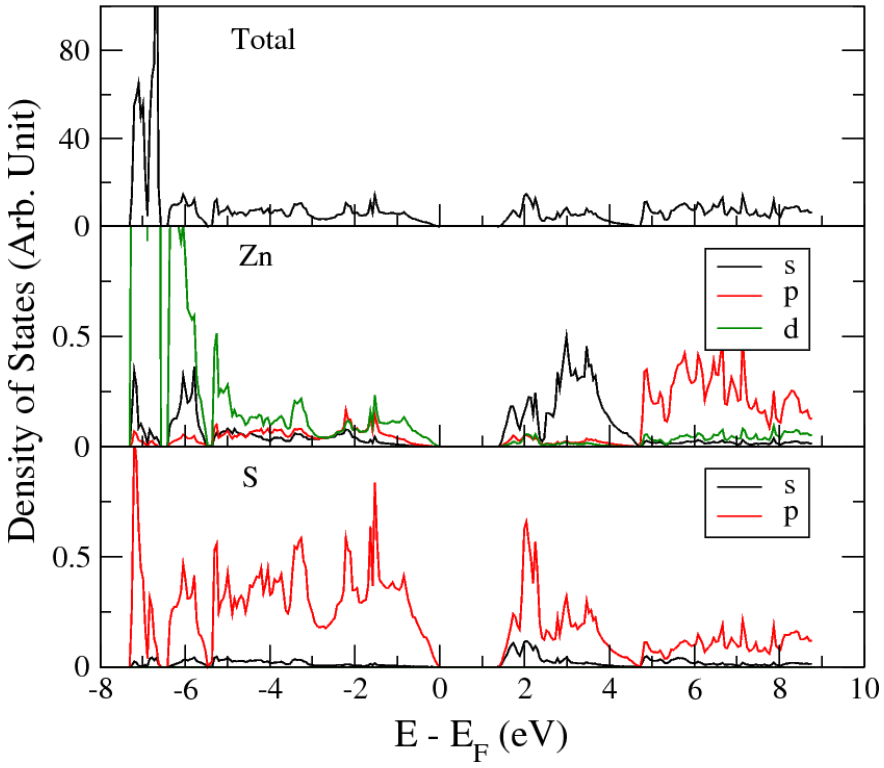
Dopant concentration: 3.1%

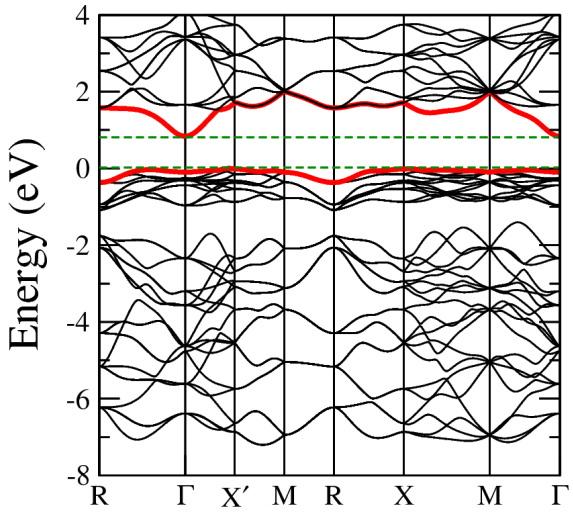
II. Results: $Fe_{1-x}Zn_xS_2$ alloys

FeS_2

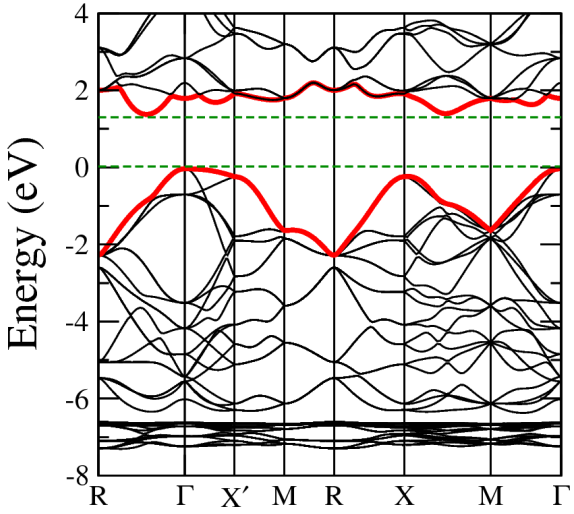


ZnS_2



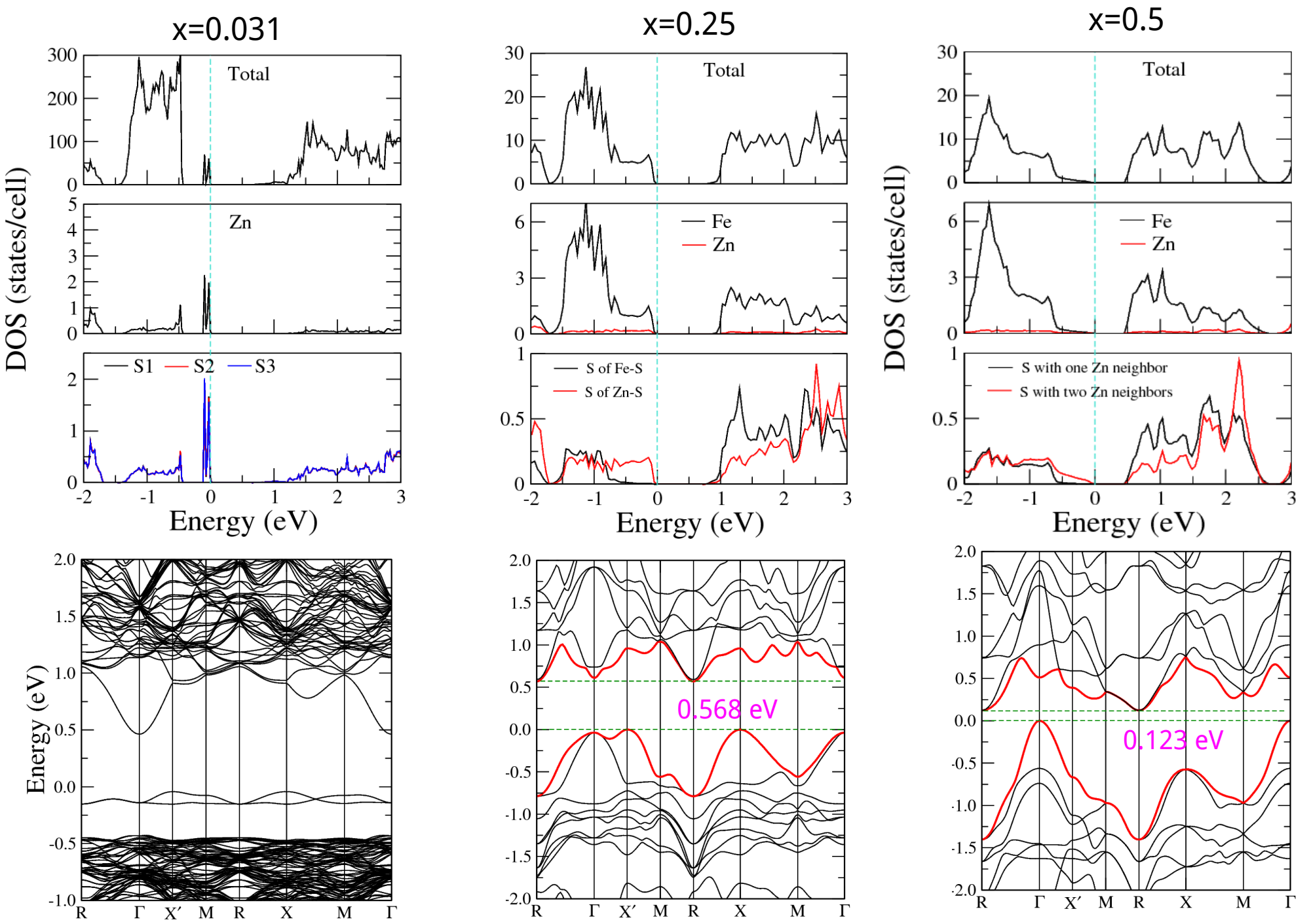


0.81 eV



1.38 eV

II. Results: $Fe_{1-x}Zn_xS_2$ alloys



III. Conclusions

1. p-type FeS_2 is difficult to be achieved. Our suggestions is to use n-type FeS_2 and p-type ZnS_2 to produce p-n junction.

2. The valence bands of $Fe_{1-x}Zn_xS_2$ alloys changes a lot with respect to pure FeS_2 and ZnS_2, which may be used to dope p-type material.