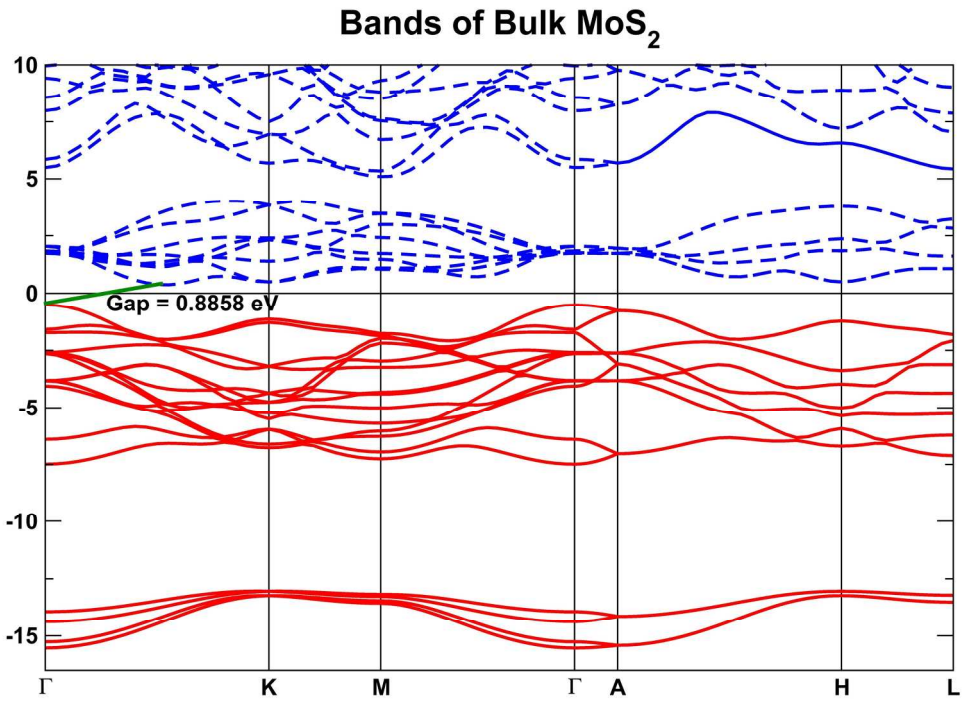
Supplementary Material

BANDS-BULK

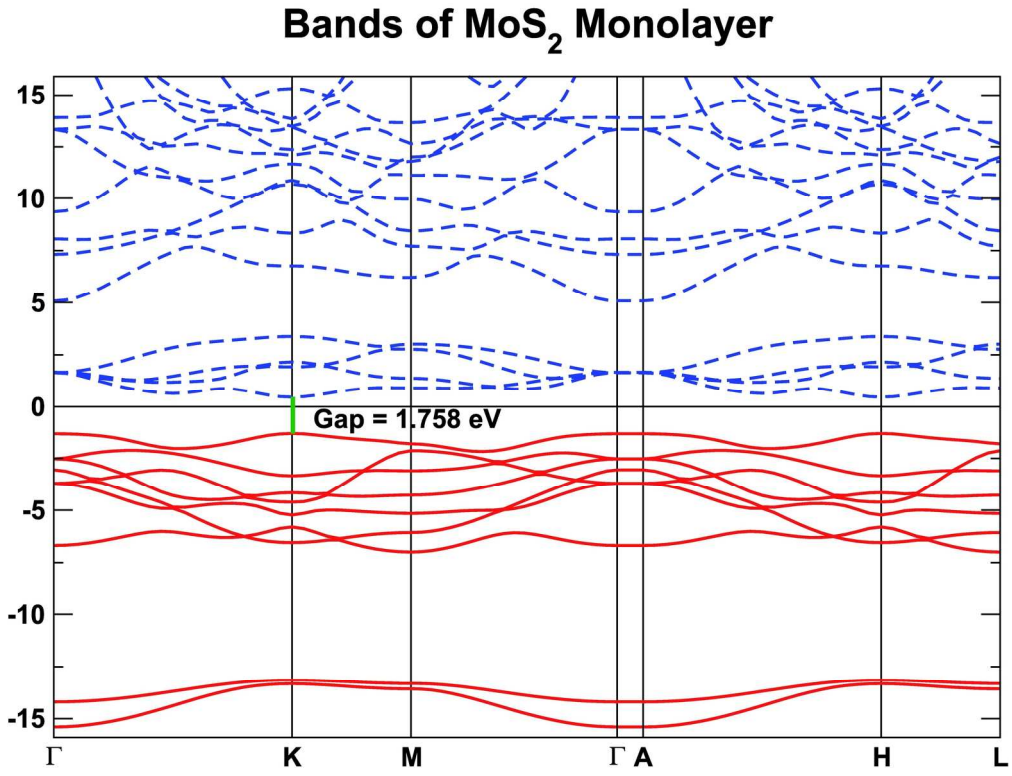
BANDS S-Mo-S

PDOS

The biggest contribution for the majority spin comes from the *3p* orbitals of the S atoms, followed by the *4d* orbitals of Mo. For the minority spin, the states just above the Fermi energy are mainly from the *4d* orbitals of the Mo and the *3d* orbitals of S atoms. As we cross the Fermi energy, the minority spin DOS goes to 0, and below that, the relative weights invert for the group of bands shown in Fig. 5, where the contribution of the *3p* orbitals from the S atoms contributes more than the *4d* orbitals of the Mo atoms



196x144mm (300 x 300 DPI)



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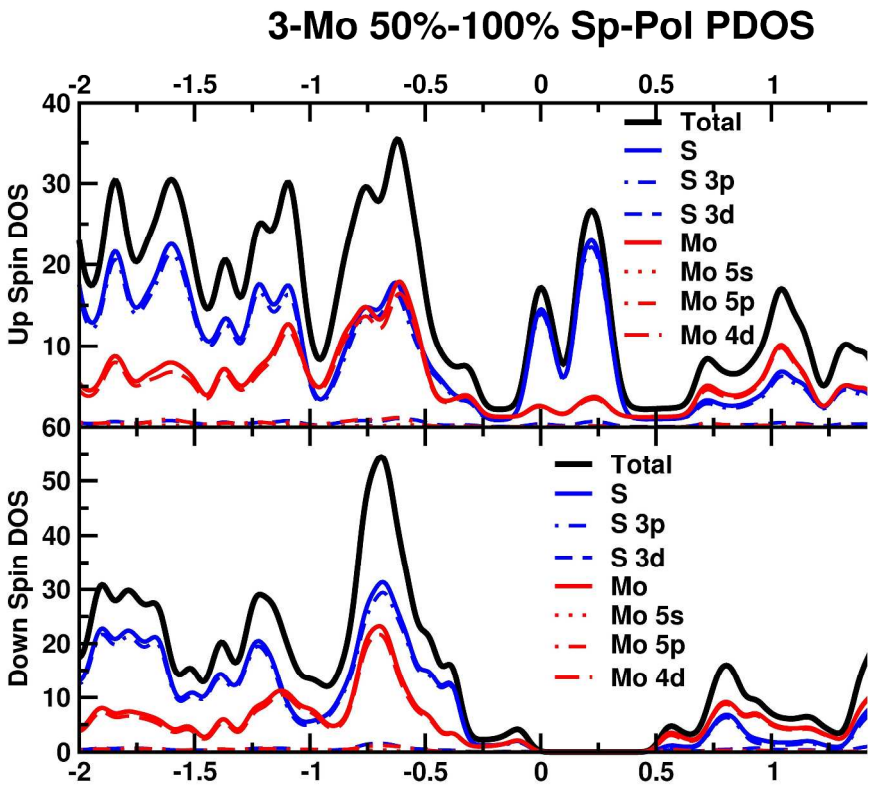
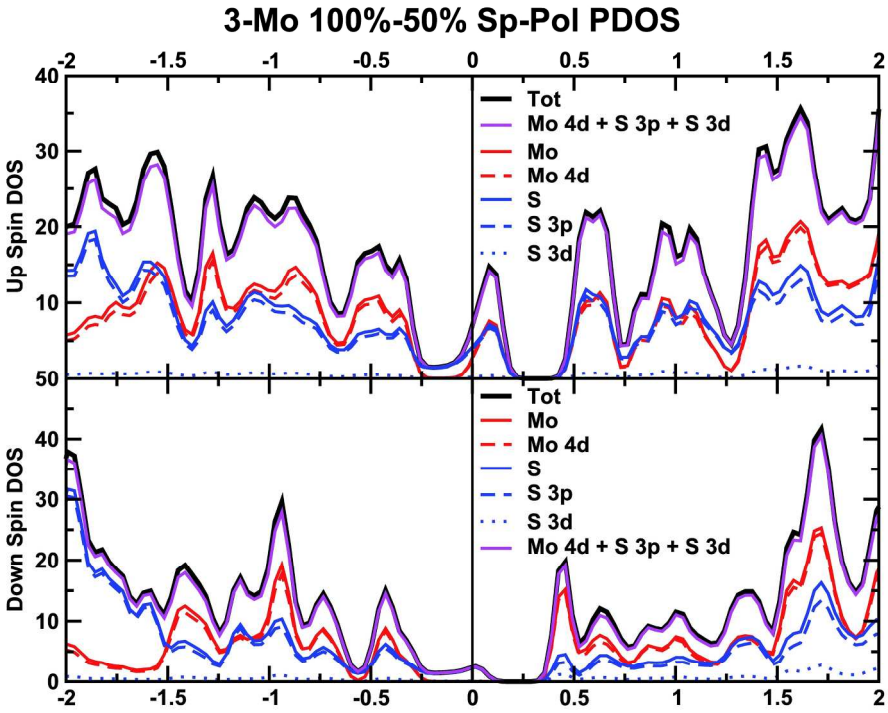
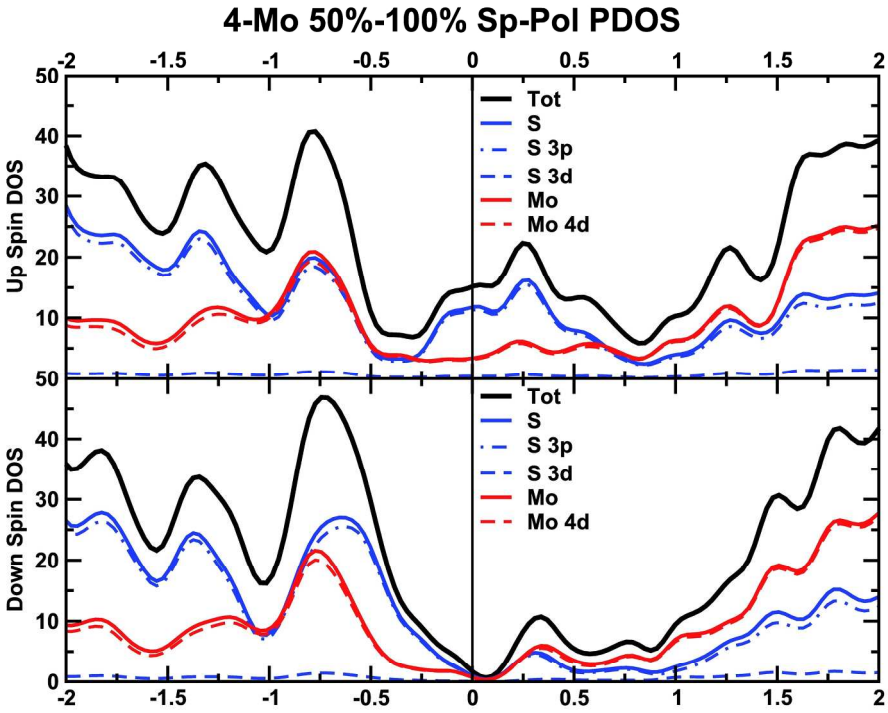


279x361mm (300 x 300 DPI)



215x166mm (300 x 300 DPI)



215x166mm (300 x 300 DPI)

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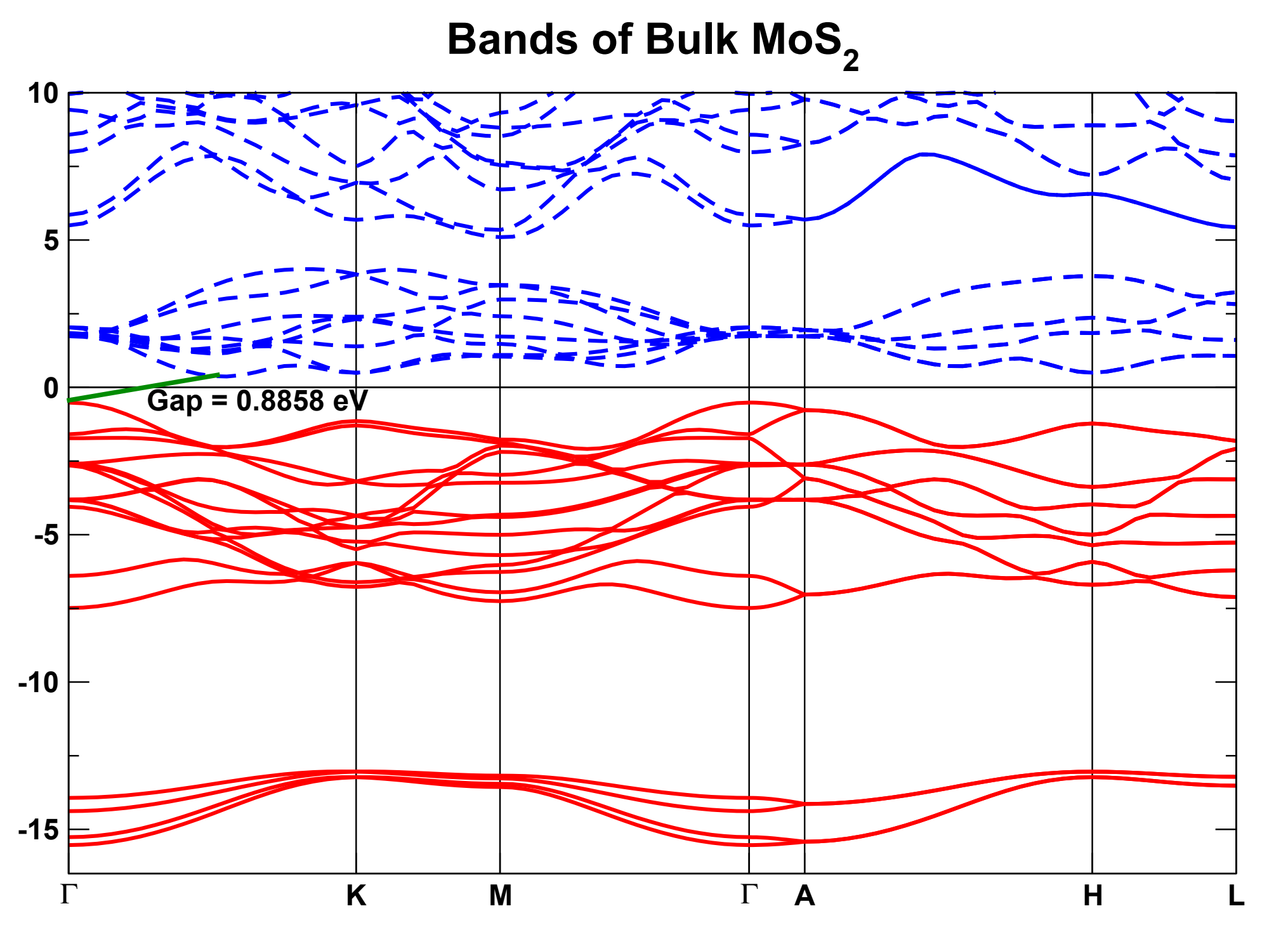
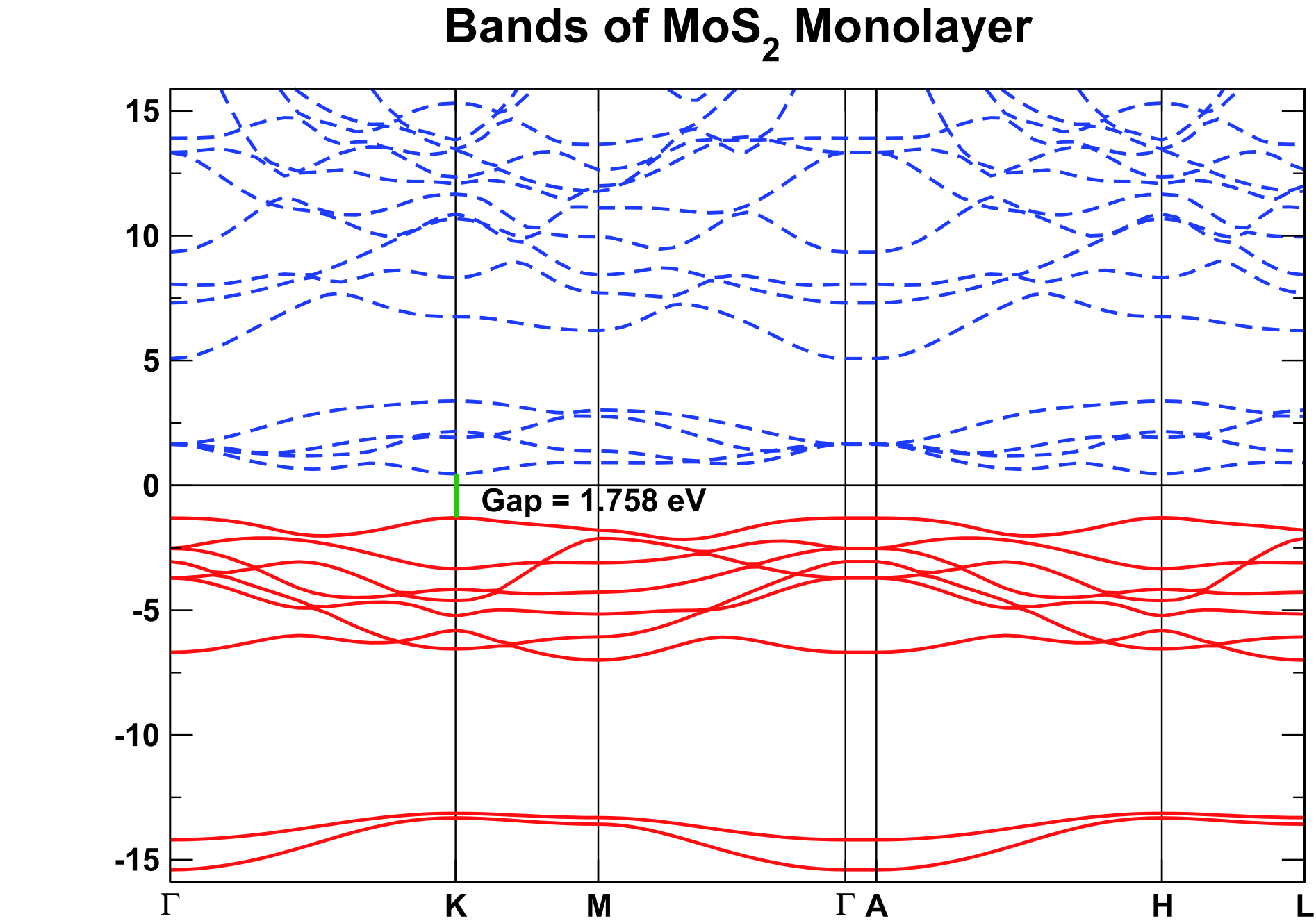
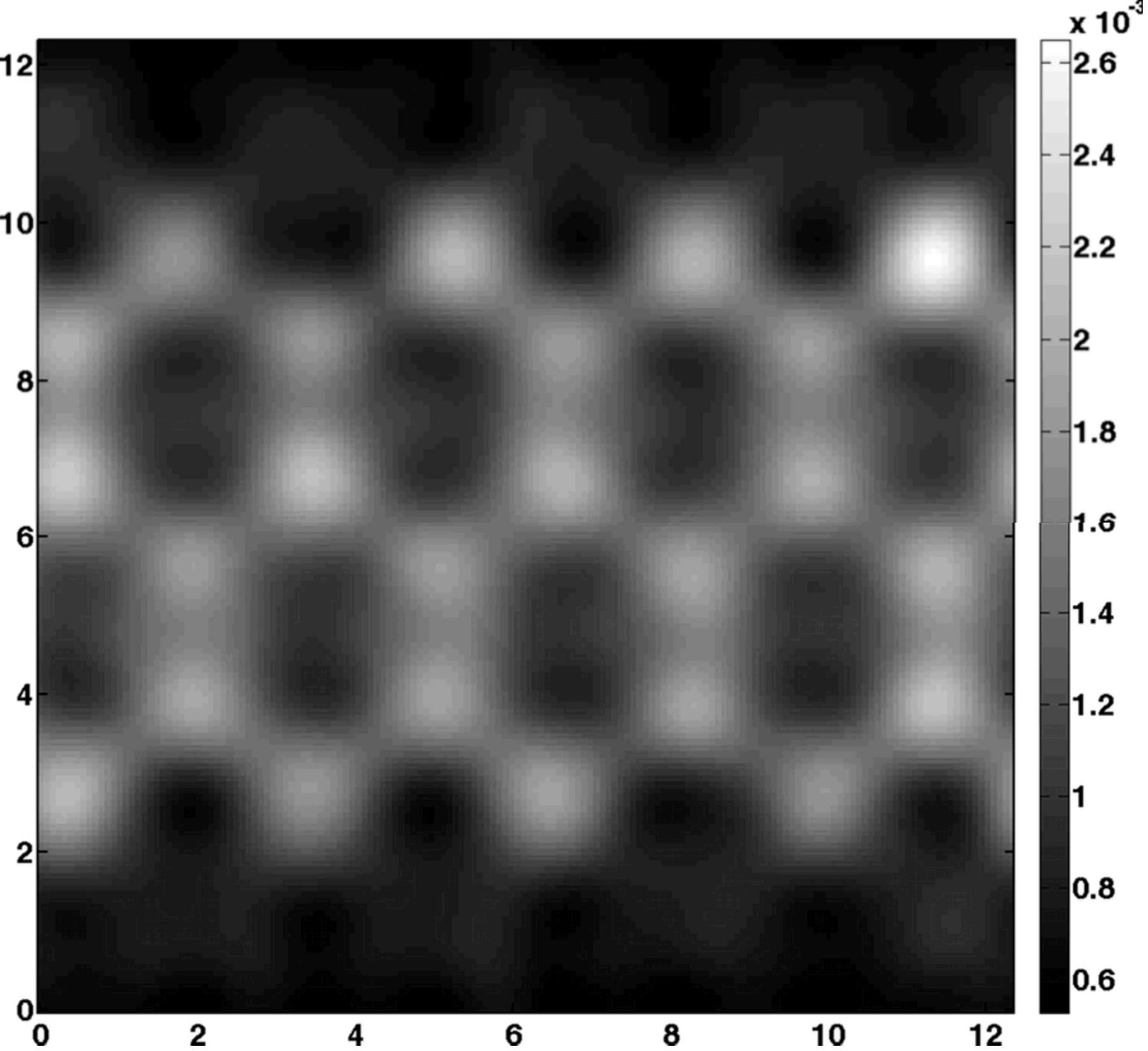

Bands of Bulk MoS2
10
5
0
-5
-10
-15
Gap = 0.8858 eV
Γ
K
M
Γ
A
H
L

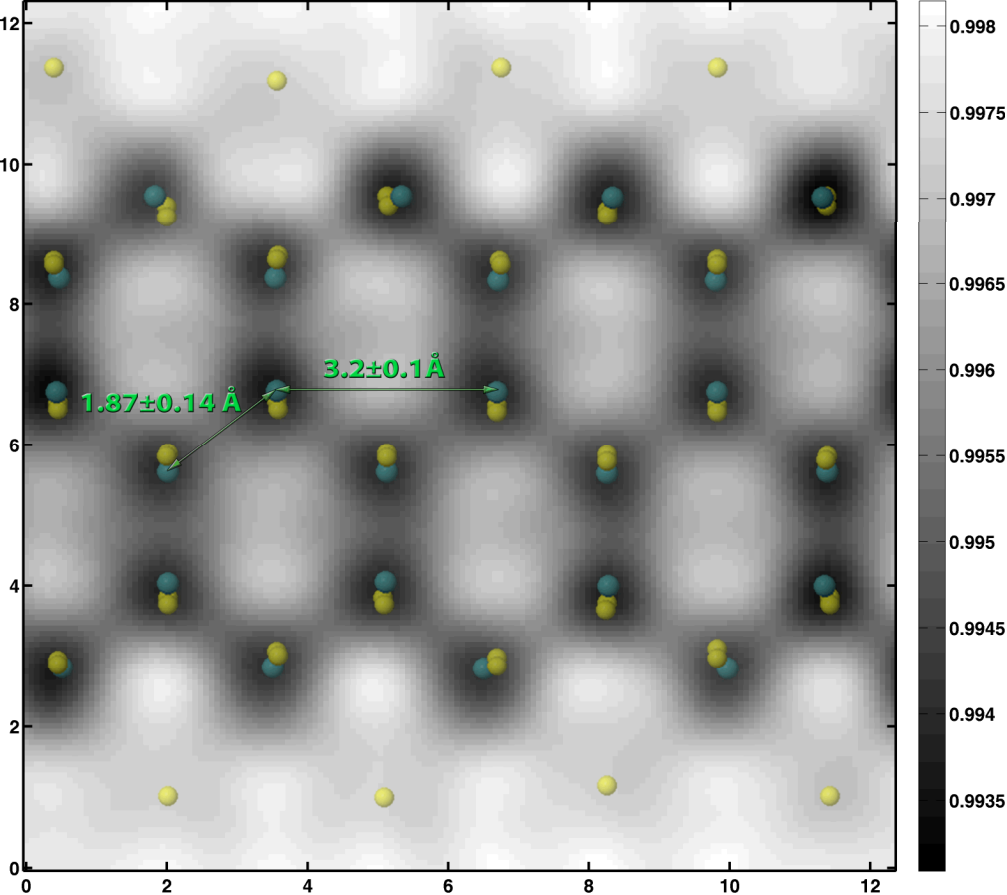
Type of file: figure
Label: Suppl2
Filename: S088429141200355Xsup002.eps


Bands of MoS2 Monolayer
15
10
5
0
-5
-10
-15
Gap = 1.758 eV
Γ
K
M
Γ
A
H
L

Type of file: figure
Label: Suppl3
Filename: S088429141200355Xsup003.tiff


x 10^-3
2.6
2.4
2.2
2
1.8
1.6
1.4
1.2
1
0.8
0.6
0
2
4
6
8
10
12

Type of file: figure
Label: Suppl4
Filename: S088429141200355Xsup004.tiff


3.2±0.1Å
1.87±0.14 Å
0
2
4
6
8
10
12
0.998
0.9975
0.997
0.9965
0.996
0.9955
0.995
0.9945
0.994
0.9935