$\varepsilon_p = 4.1$

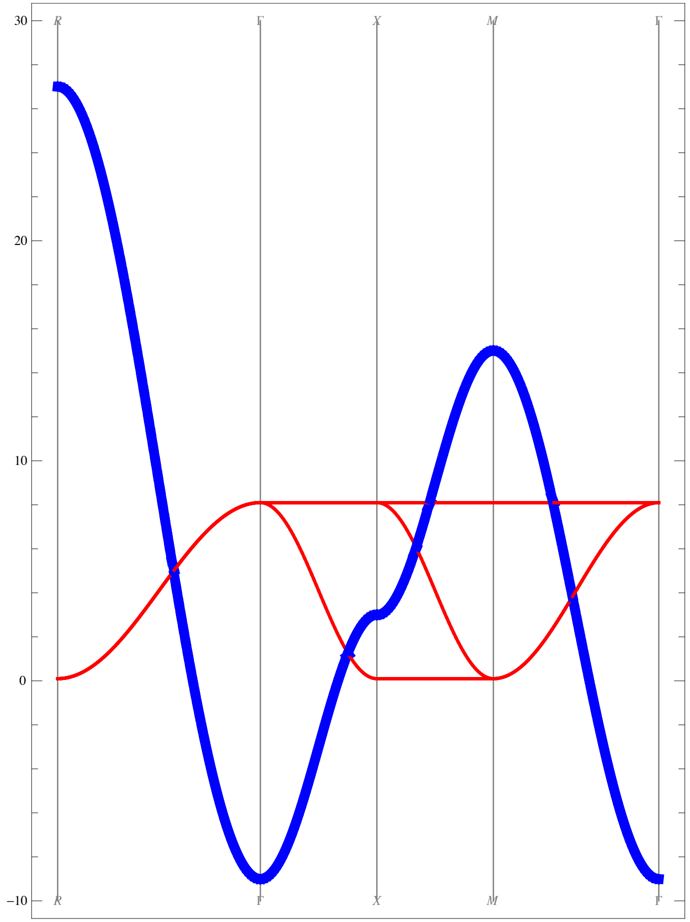
$\varepsilon_s = 9$

$ss\sigma = -3$

$pp\sigma = 2$

$sp\sigma = 0$ (No s-p mixing)

$\zeta = 0$ (No SOC)



$\varepsilon_p = 4.1$

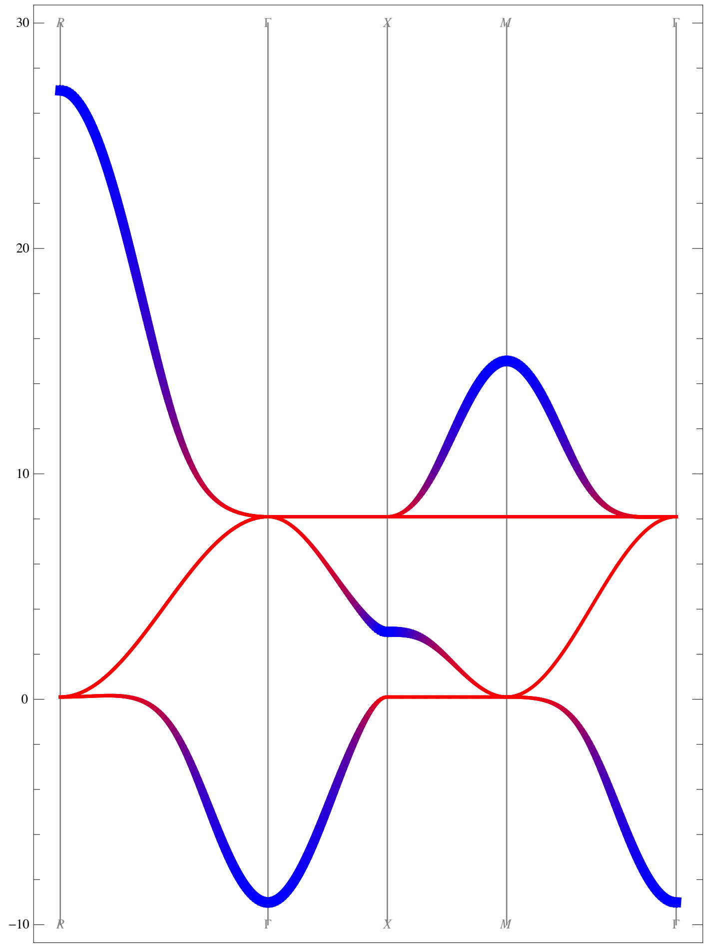
$\varepsilon_s = 9$

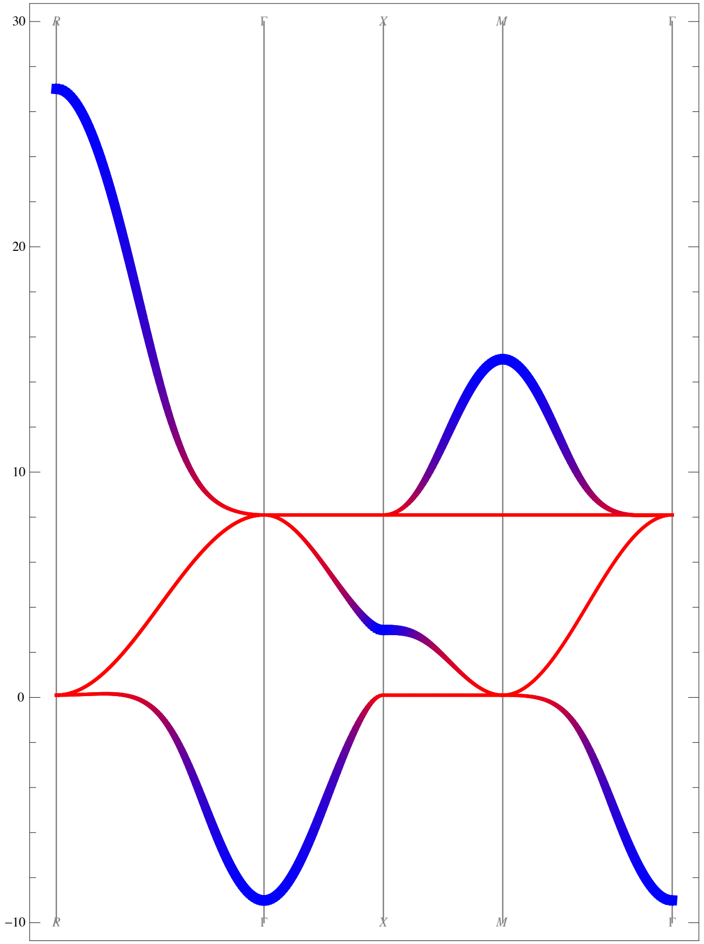
$ss\sigma = -3$

$pp\sigma = 2$

$sp\sigma = 2$

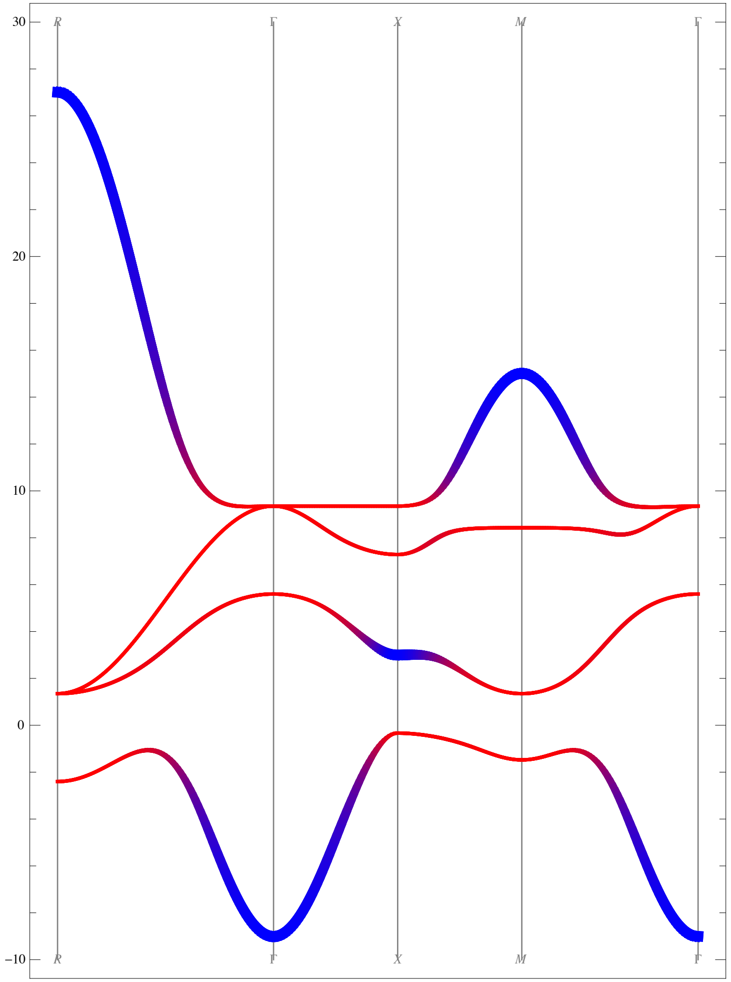
$\zeta = 0$ (No SOC)

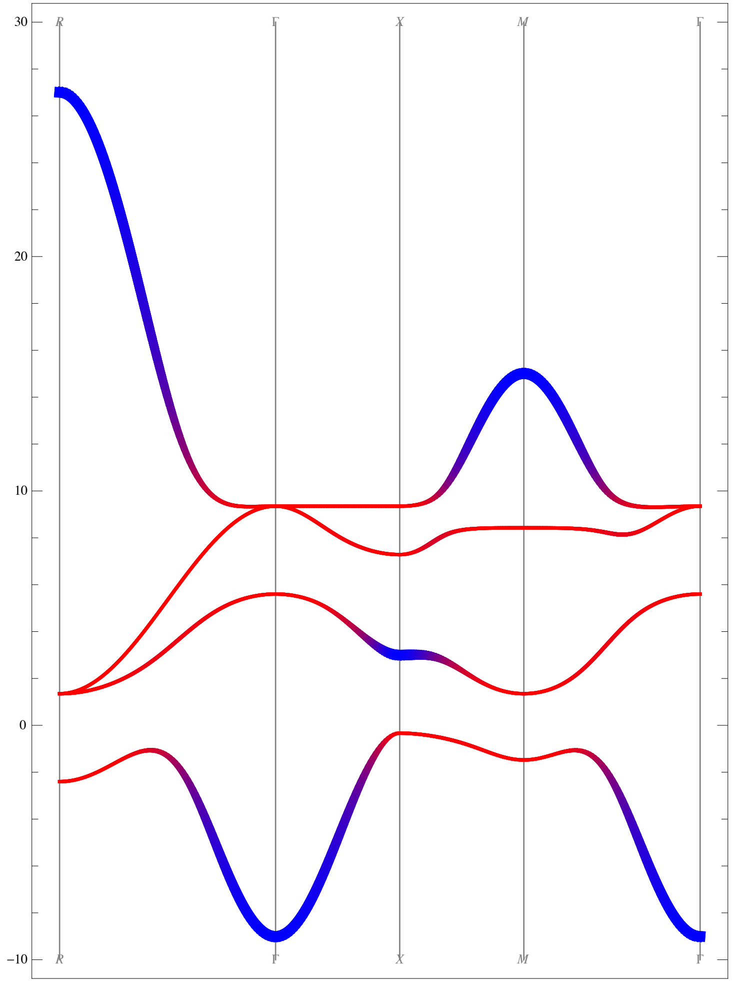




One can see on the left: the s-p mixing creates hybridization gaps between the s and p band. However, at high symmetry points (R={1,1,1}, M={1,1,0}, X={1,0,0} and Γ={0,0,0}) the s and p band do not mix by symmetry. The system without spin-orbit coupling therefore is metallic.

$\varepsilon_p = 4.1$
$\varepsilon_s = 9$
$ss\sigma = -3$
$pp\sigma = 2$
$sp\sigma = 2$
$\zeta = 2.5$





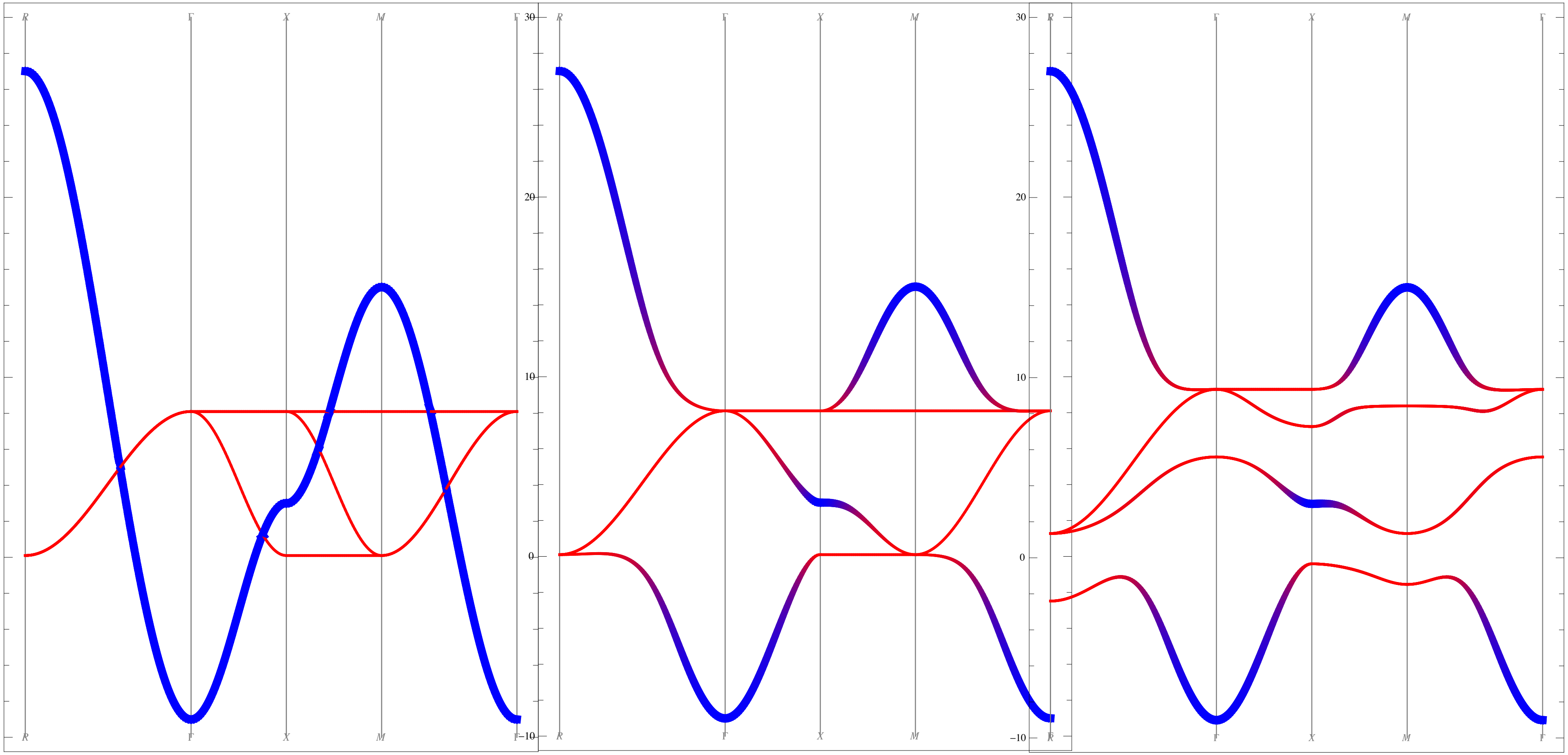
We have now included spin-orbit coupling and this splits the p-bands into a j=1/2 and j=3/2 state. Now a single band splits off and if there is a filling of 2 electrons per site this band is fully occupied and the system is an insulator.

The gap, which is of indirect type (maximum of the valance band is at X, minimum of the conduction band at M or/and R) is between states of p character.

$\varepsilon_p = 4.1$
$\varepsilon_s = 9$
ssσ = -3
ppσ = 2
spσ = 0 (No s-p mixing)
ζ = 0 (No SOC)

$\varepsilon_p = 4.1$
$\varepsilon_s = 9$
ssσ = -3
ppσ = 2
spσ = 2
ζ = 0 (No SOC)

$\varepsilon_p = 4.1$
$\varepsilon_s = 9$
ssσ = -3
ppσ = 2
spσ = 2
ζ = 2.5



We now can test if the state with two electrons per site is a topological insulator or not. For cubic systems the number that distinguishes topological trivial case from a topological nontrivial case is calculated as the product of the parity of the occupied wave functions at Γ, X, M, and R. If +1, then the system is trivial and if -1, the system is topological.

We can make the following parity table

	s	**p**
Γ	1	-1
X	1	-1
M	1	-1
R	1	-1

Since we now consider an electron filling of 2, we only need to consider the parities of the single filled band. At Γ, the band is blue (s-orbital). Therefore the parity is +1. At X, p-character (red), therefore parity is -1. At M, p-character (red), parity is -1. At R, again p-character, parity is -1. So, we now need to take the product of these parities (+1 * -1 * -1 * -1). This gives a total of -1. Therefore, the system above is thus topological - non-trivial.