# Topological Band Theory

*Topology is a branch of mathematics concerned with geometrical properties that are insensitive to smooth deformations.*

Based on lectures and notes
from Charles L. Kane

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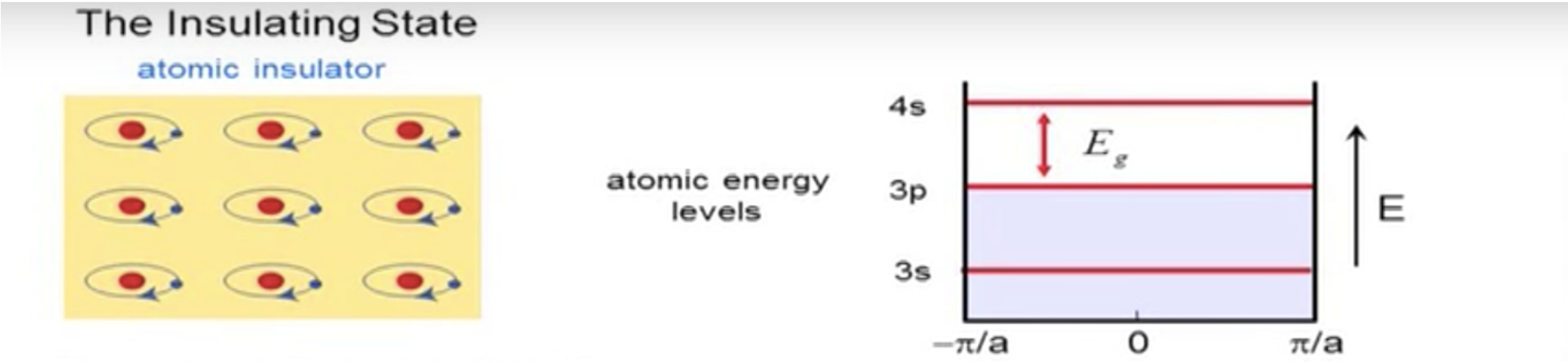
A central role of condensed matter physics → characterize phases of matter

Phases like magnets and superconductors → spontaneous symmetry breaking

Quantum Hall state → No symmetry breaking ! The properties are consequences of the topological structure of the quantum state.

# Topology vs. Integer Quantum Hall Effect



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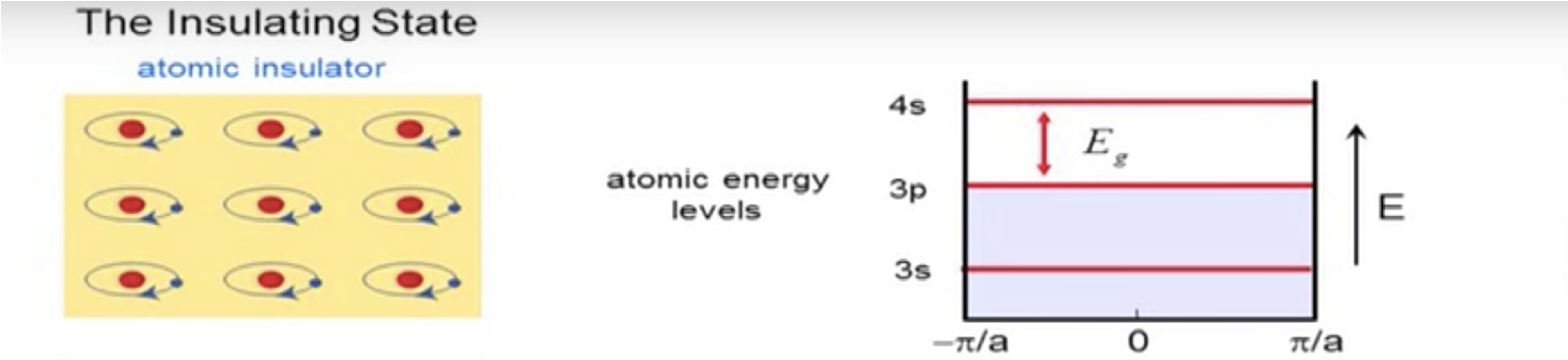
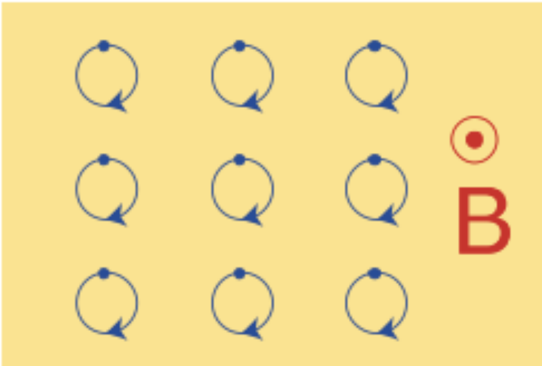
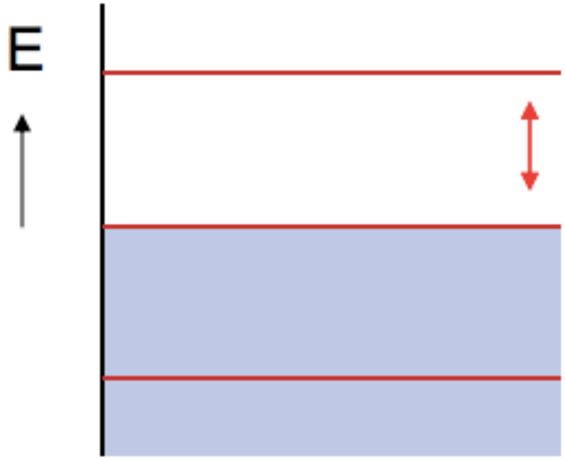



# Topology vs. Integer Quantum Hall Effect

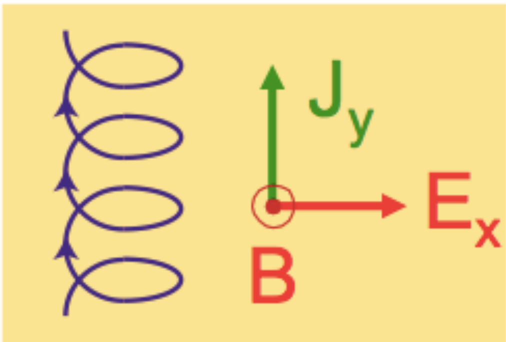
Quantum Hall Effect → Energy gap, but not an insulator !



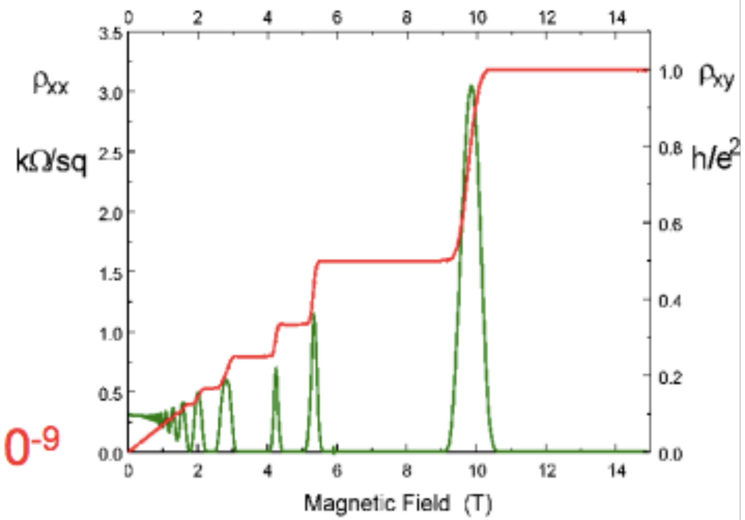

$$E_{gap} = \hbar\omega_c$$

Quantized Hall conductivity : $J_y = \sigma_{xy} E_x$




$$\sigma_{xy} = n \frac{e^2}{h}$$

Integer accurate to $10^{-9}$




Similarly, Topological Insulators → Bulk energy gap, but conducting surface

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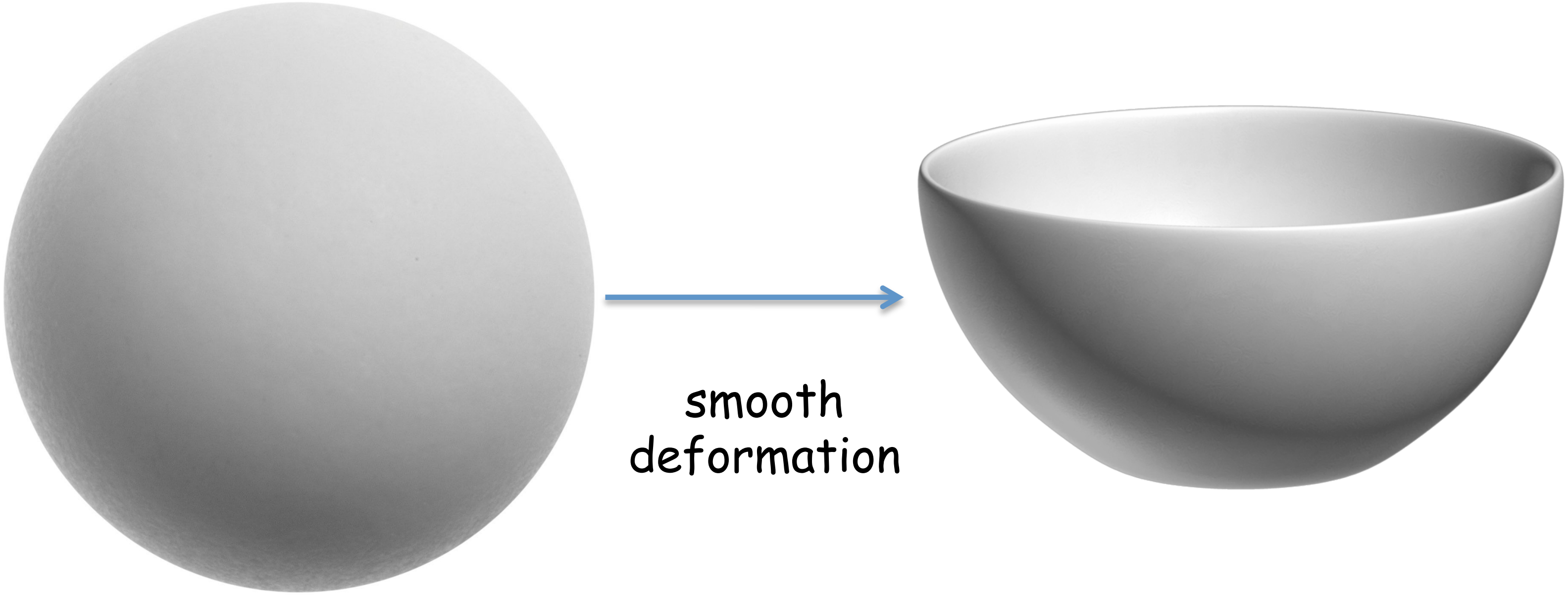

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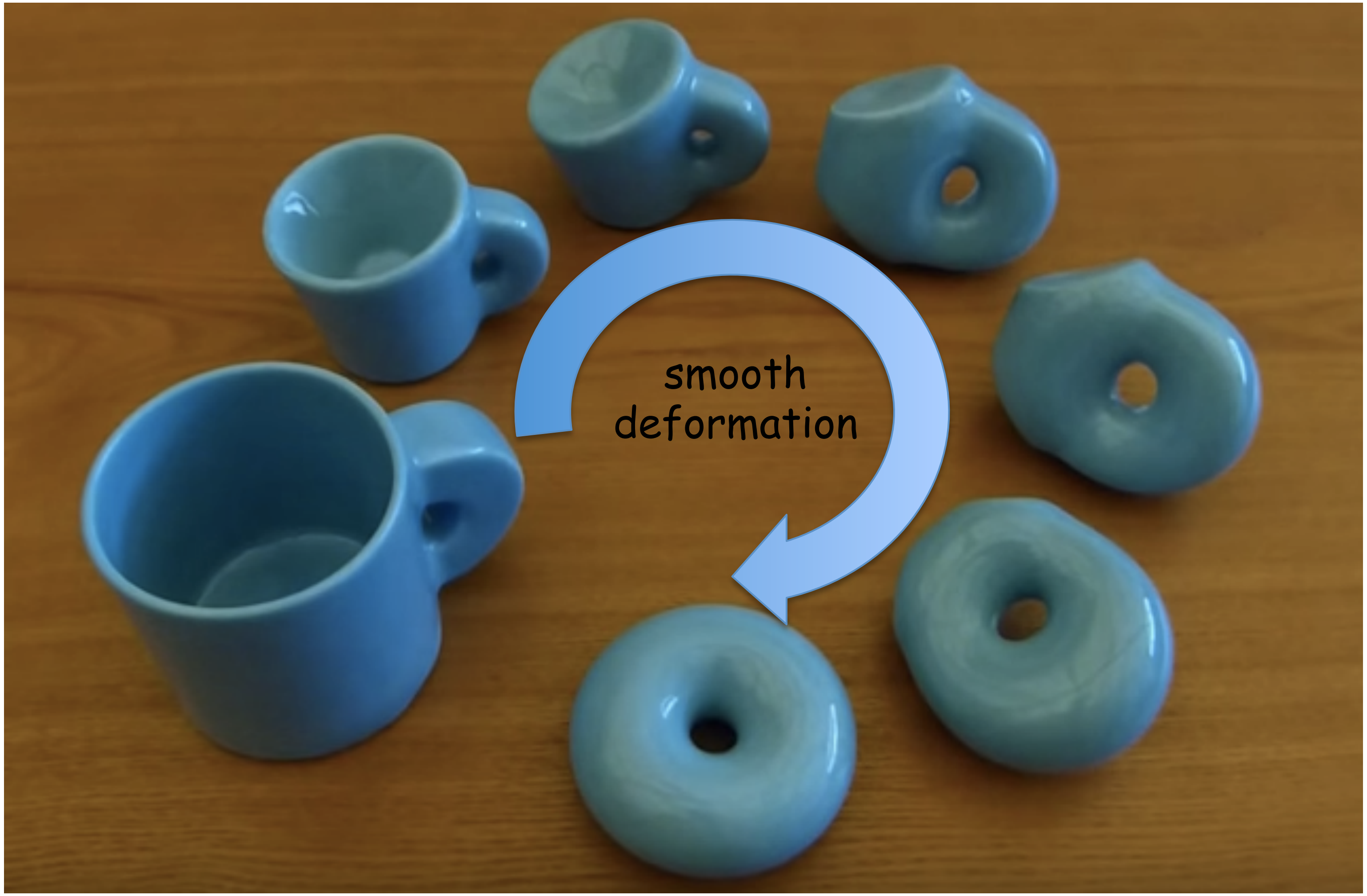

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Credit: wikimedia

# <u>Topology</u>

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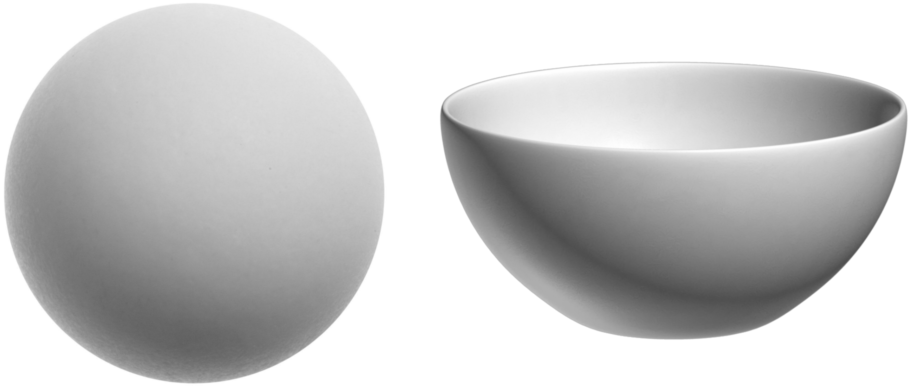

A sphere and a doughnut are distinguished by an integer topological invariant called the *genus*, *g*, which is essentially the number of holes.

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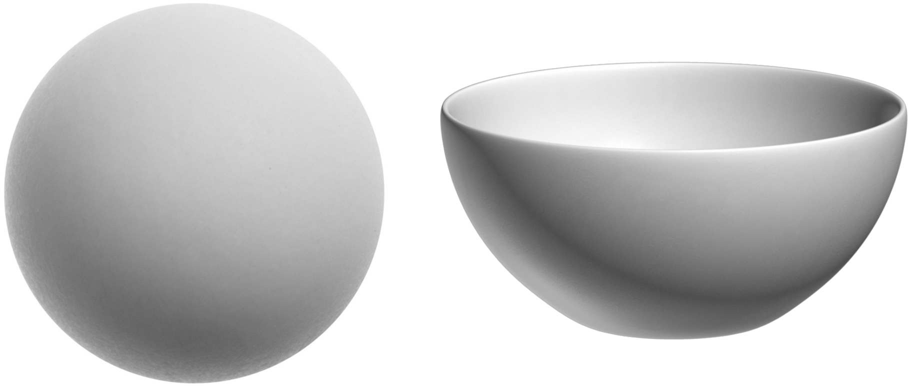

g = 0

g = 1

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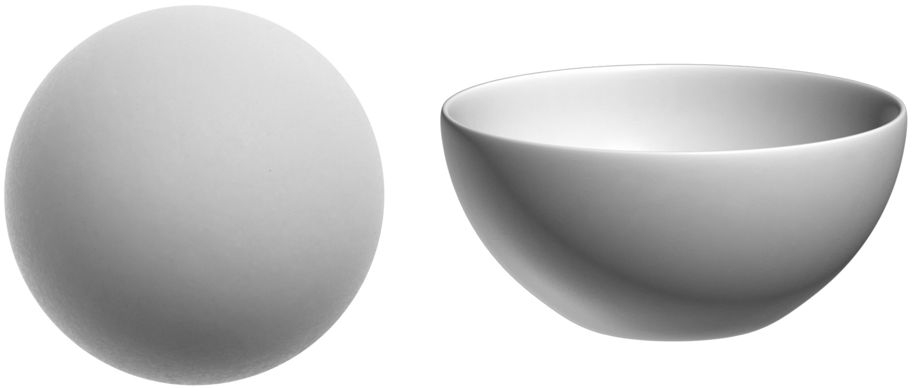

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A sphere and a doughnut are distinguished by an integer topological invariant called the *genus*, $g$, which is essentially the number of holes. Since an integer cannot change smoothly, surfaces with different genus cannot be deformed into one another, and are said to be topologically distinct.

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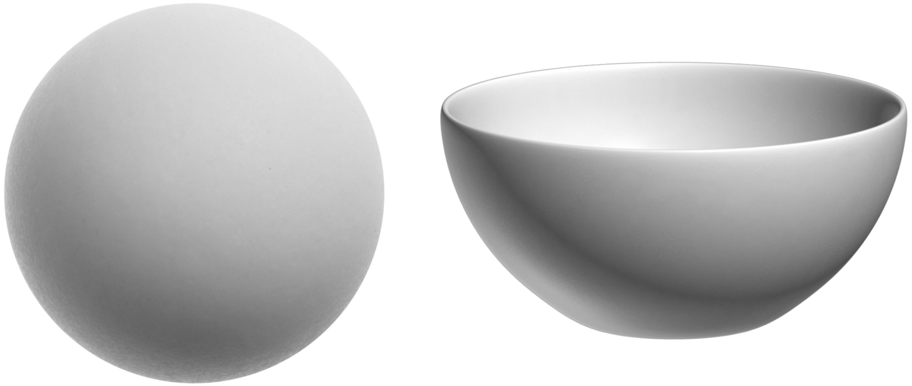

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A sphere and a doughnut are distinguished by an integer topological invariant called the *genus*, $g$, which is essentially the number of holes. Since an integer cannot change smoothly, surfaces with different genus cannot be deformed into one another, and are said to be topologically distinct. Surfaces that can be deformed into one another are topologically equivalent.

# Topology

In band theory, insulators are equivalent if they can be changed into one another by slowly changing the Hamiltonian, such that the system always remains in the ground state.

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Insulators are topologically equivalent if there exists an adiabatic path connecting them along which the *energy gap remains finite.*

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Insulators are topologically equivalent if there exists an adiabatic path connecting them along which the *energy gap remains finite.*

It then follows → connecting topologically inequivalent insulators necessarily involves a phase transition, in which the energy gap vanishes.

# Topology

Let's look back at the tightbinding example, wherein we calculated topologically non-trivial surface states.

We will change the band structure (i.e. smooth deformation) and monitor if they fall in same "genus"

The fingerprint of this is the surface state that remains linear close to $\Gamma$.

# Topologically equivalent phases

In last lecture → a tightbinding model on a square lattice with one s and three p orbitals

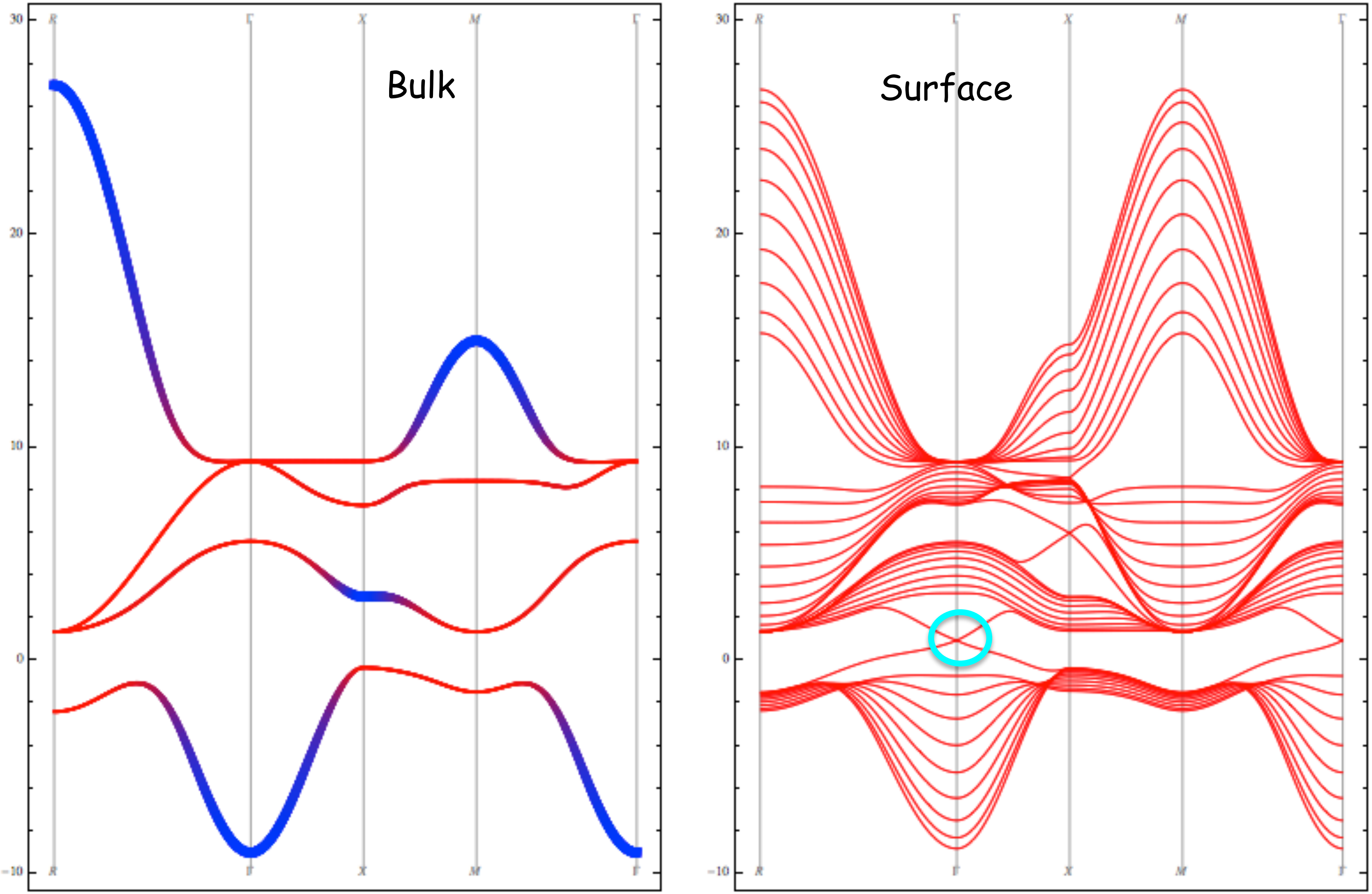
$$
H = \begin{pmatrix}
\epsilon p + pp\sigma \left(e^{i\pi\kappa x} + e^{-i\pi\kappa x}\right) & 0 & 0 & sp\sigma \left(e^{i\pi\kappa x} - e^{-i\pi\kappa x}\right) \\
0 & \epsilon p + pp\sigma \left(e^{i\pi\kappa y} + e^{-i\pi\kappa y}\right) & 0 & sp\sigma \left(e^{i\pi\kappa y} - e^{-i\pi\kappa y}\right) \\
0 & 0 & \epsilon p + pp\sigma \left(e^{i\pi\kappa z} + e^{-i\pi\kappa z}\right) & sp\sigma \left(e^{i\pi\kappa z} - e^{-i\pi\kappa z}\right) \\
sp\sigma \left(-e^{i\pi\kappa x} + e^{-i\pi\kappa x}\right) & sp\sigma \left(-e^{i\pi\kappa y} + e^{-i\pi\kappa y}\right) & sp\sigma \left(-e^{i\pi\kappa z} + e^{-i\pi\kappa z}\right) & \epsilon s + ss\sigma \left(e^{i\pi\kappa x} + e^{-i\pi\kappa x} + e^{i\pi\kappa y} + e^{-i\pi\kappa y} + e^{i\pi\kappa z} + e^{-i\pi\kappa z}\right)
\end{pmatrix}
$$

# Topologically equivalent phases

In last lecture → a tightbinding model on a square lattice with one s and three p orbitals

$$H_{SOC} = \xi \begin{pmatrix} 0 & \frac{i}{2} & 0 & 0 & 0 & 0 & -\frac{1}{2} & 0 \\ -\frac{i}{2} & 0 & 0 & 0 & 0 & 0 & -\frac{i}{2} & 0 \\ 0 & 0 & 0 & 0 & \frac{1}{2} & \frac{i}{2} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{1}{2} & 0 & 0 & -\frac{i}{2} & 0 & 0 \\ 0 & 0 & -\frac{i}{2} & 0 & \frac{i}{2} & 0 & 0 & 0 \\ -\frac{1}{2} & \frac{i}{2} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$

# Topologically equivalent phases



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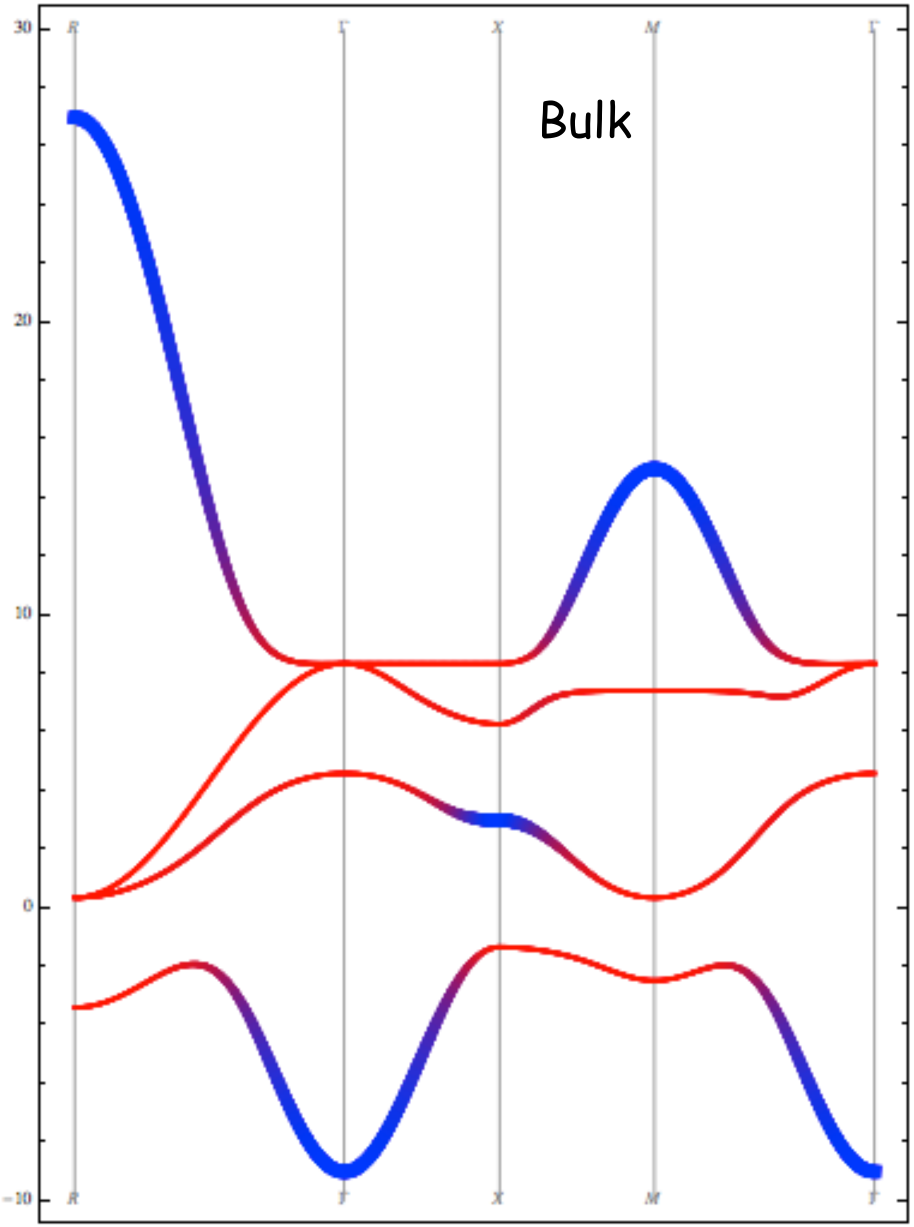


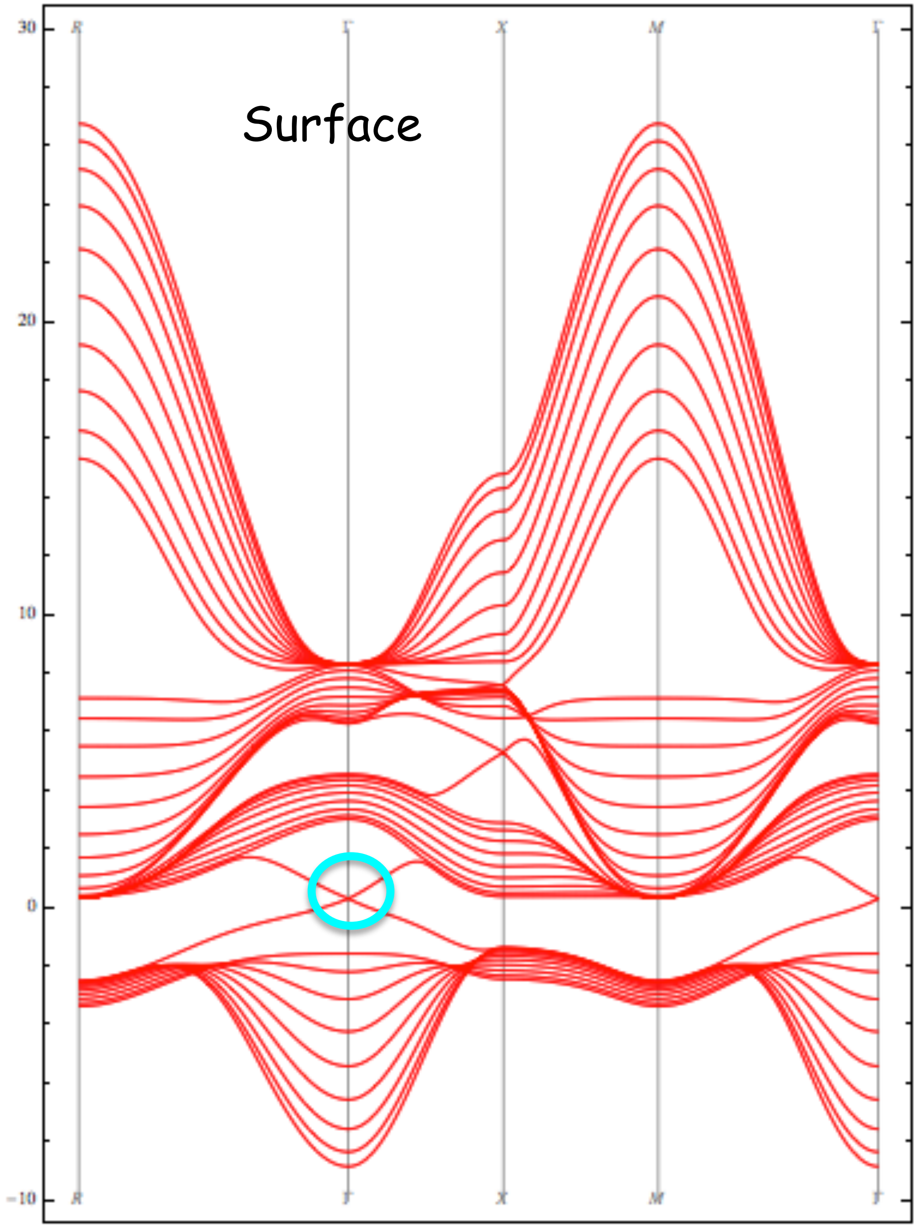

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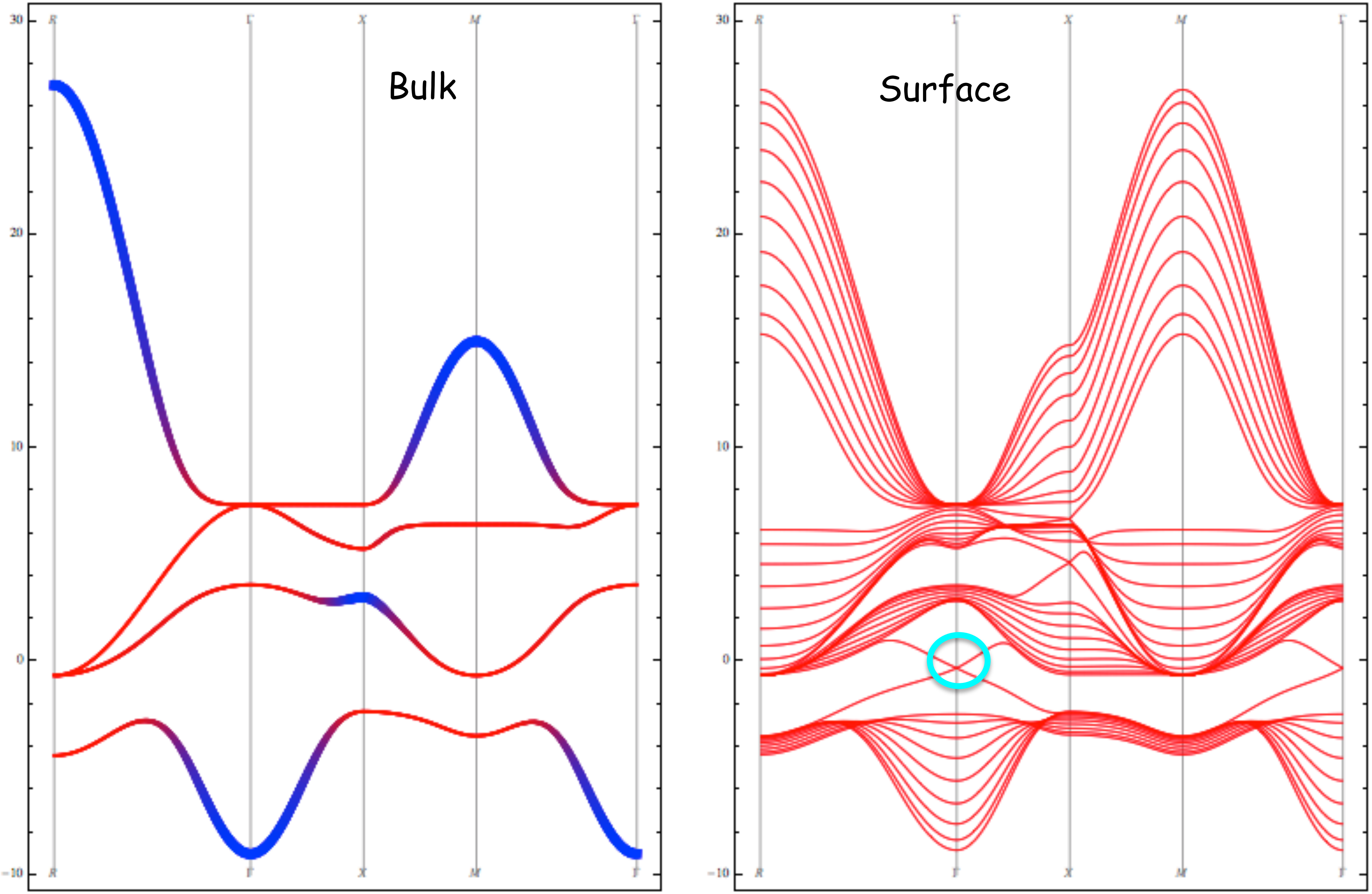

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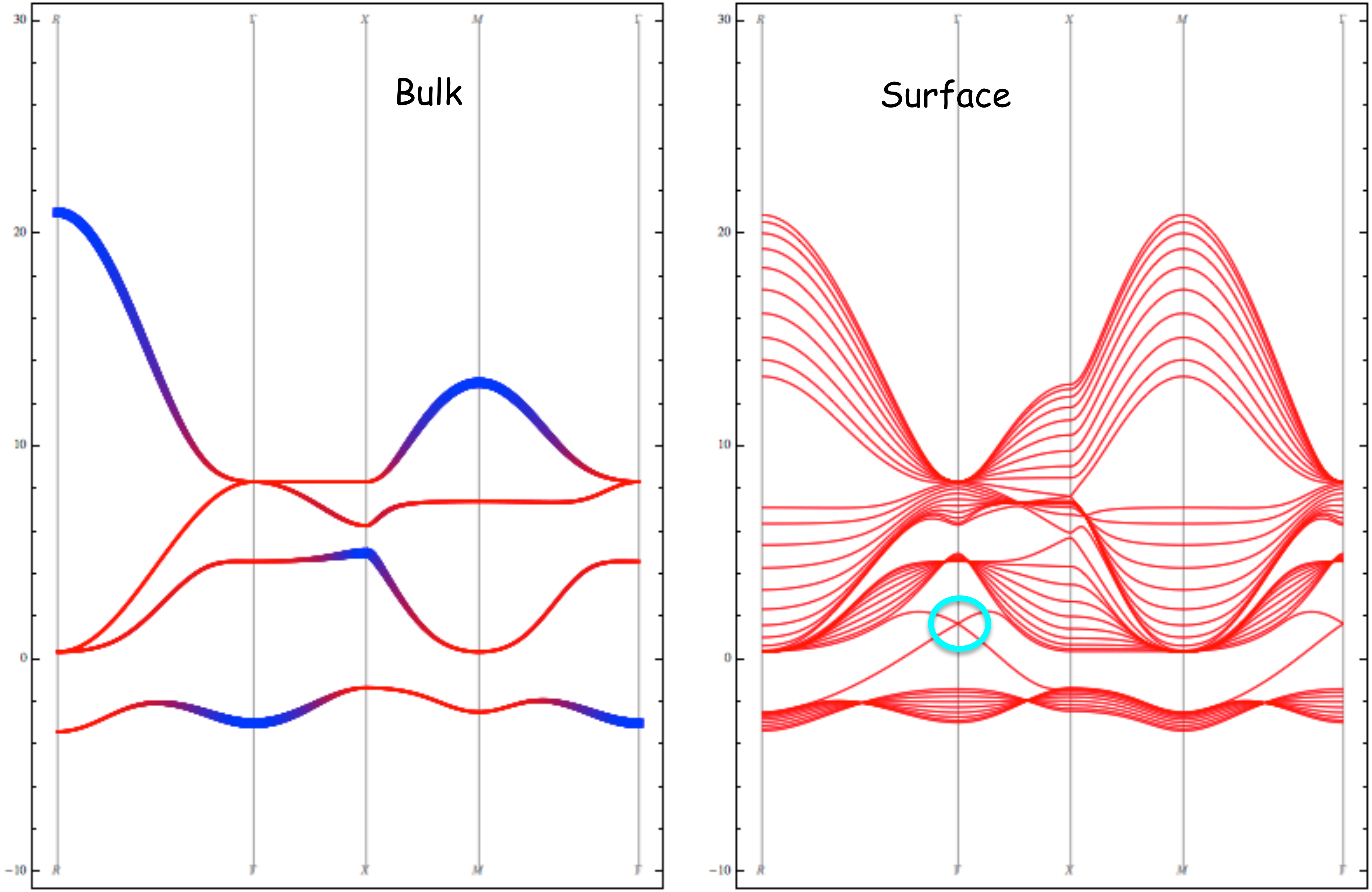

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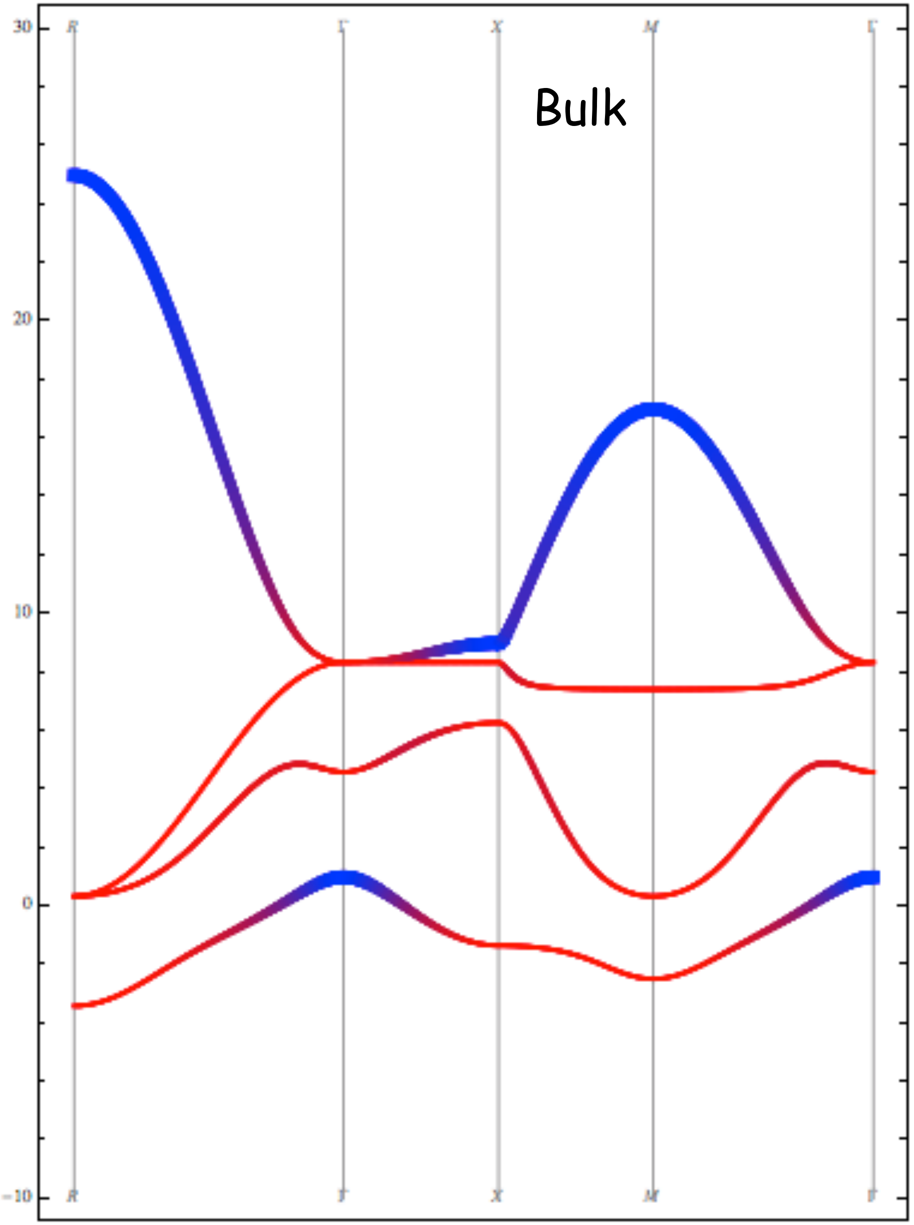


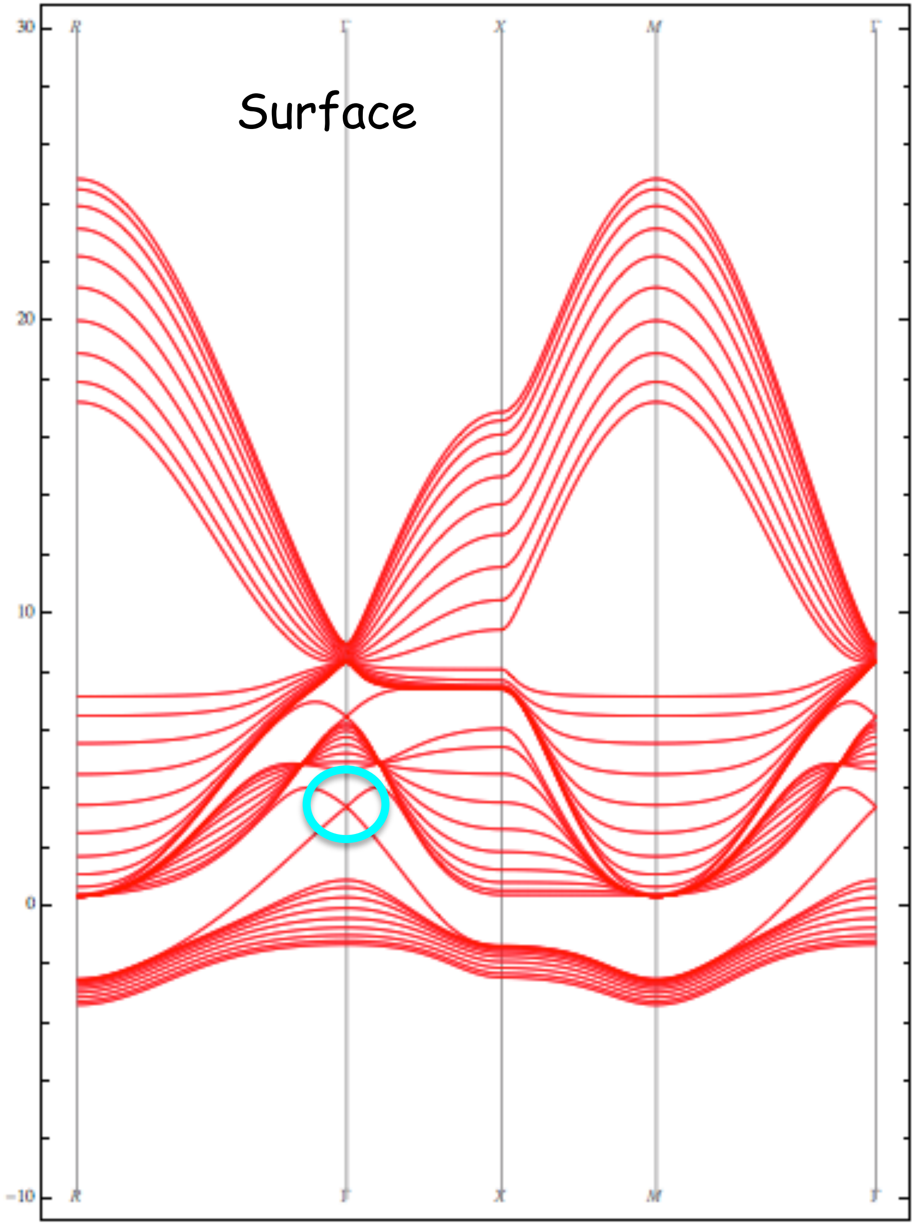

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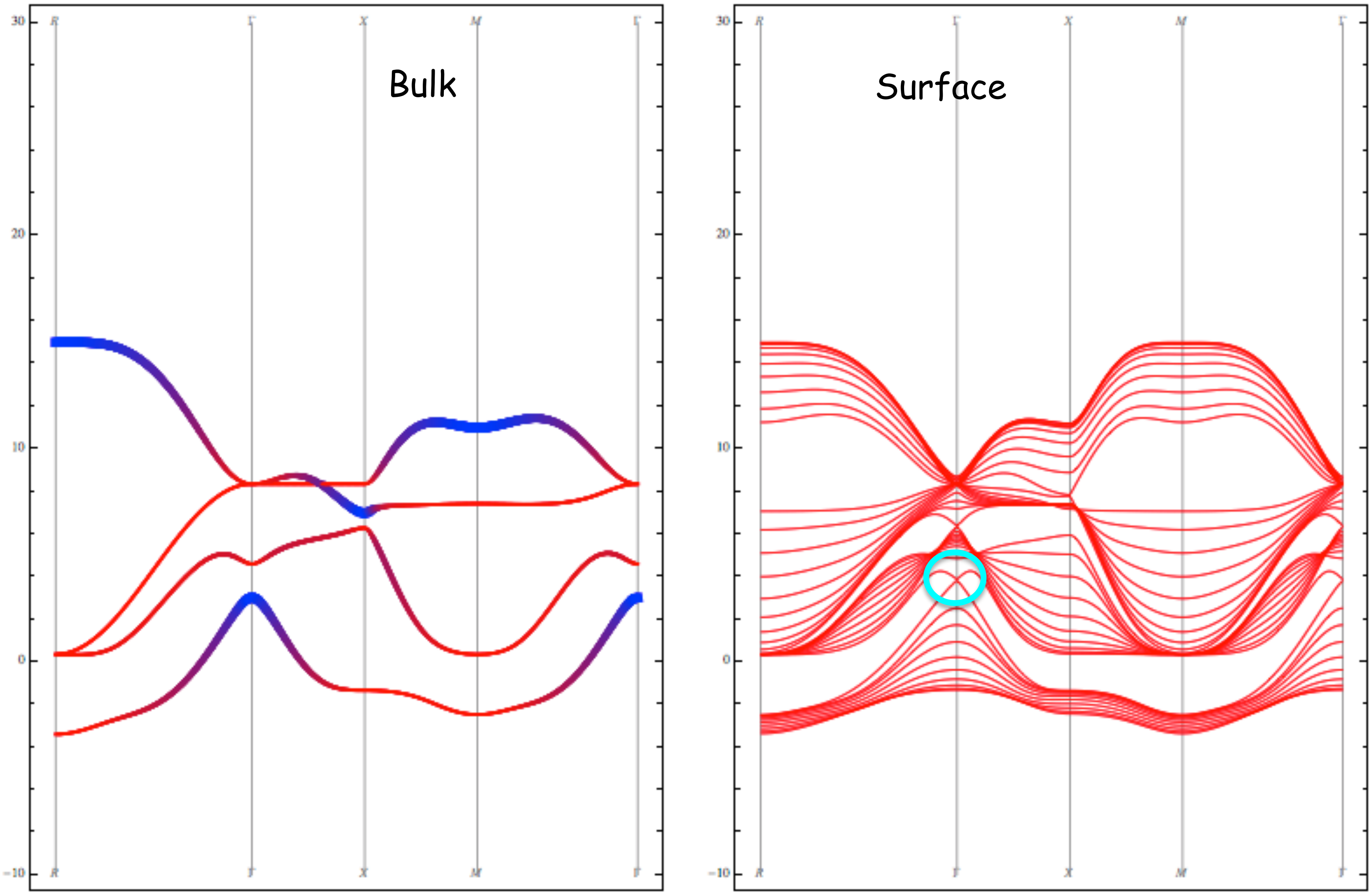

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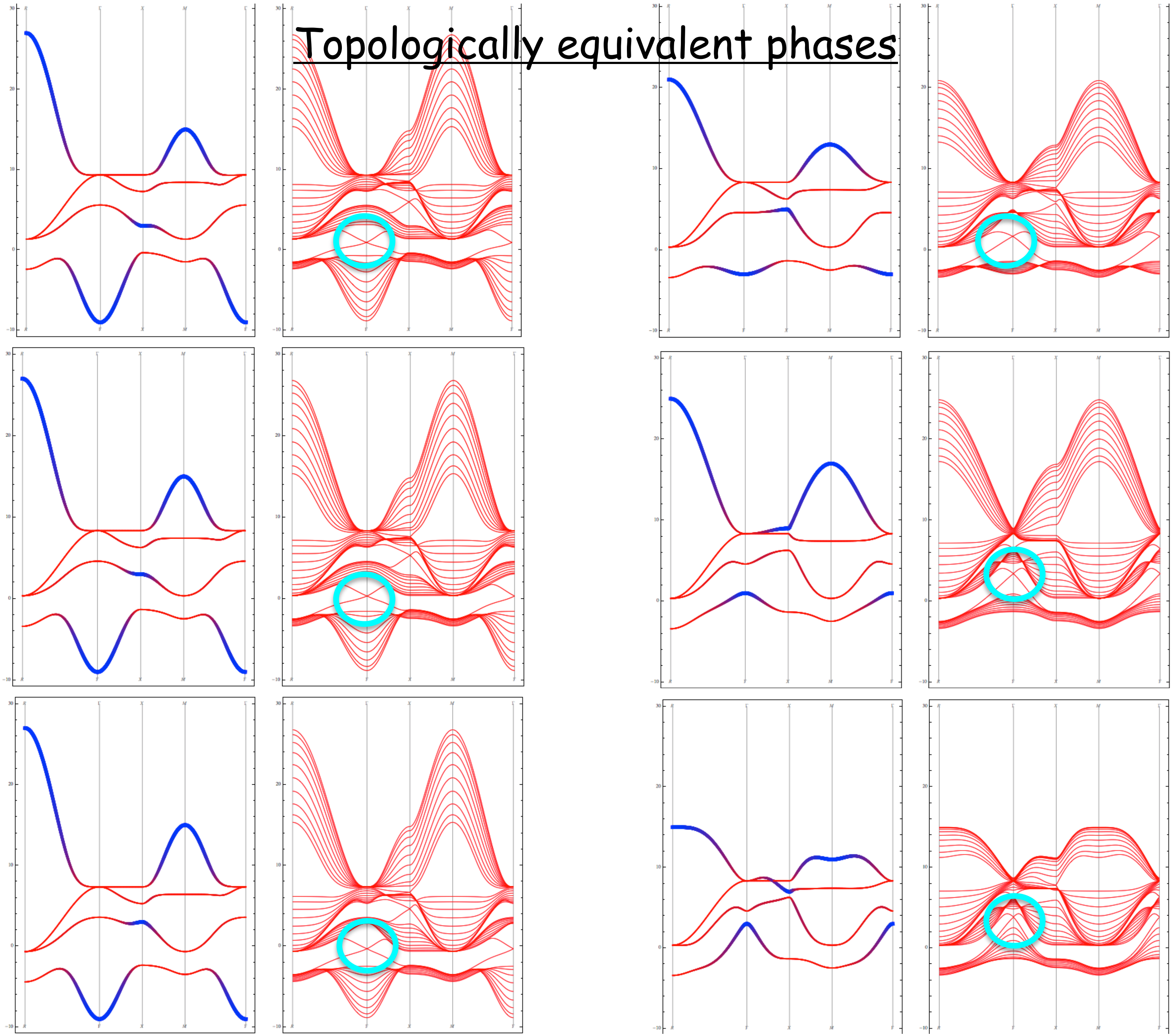
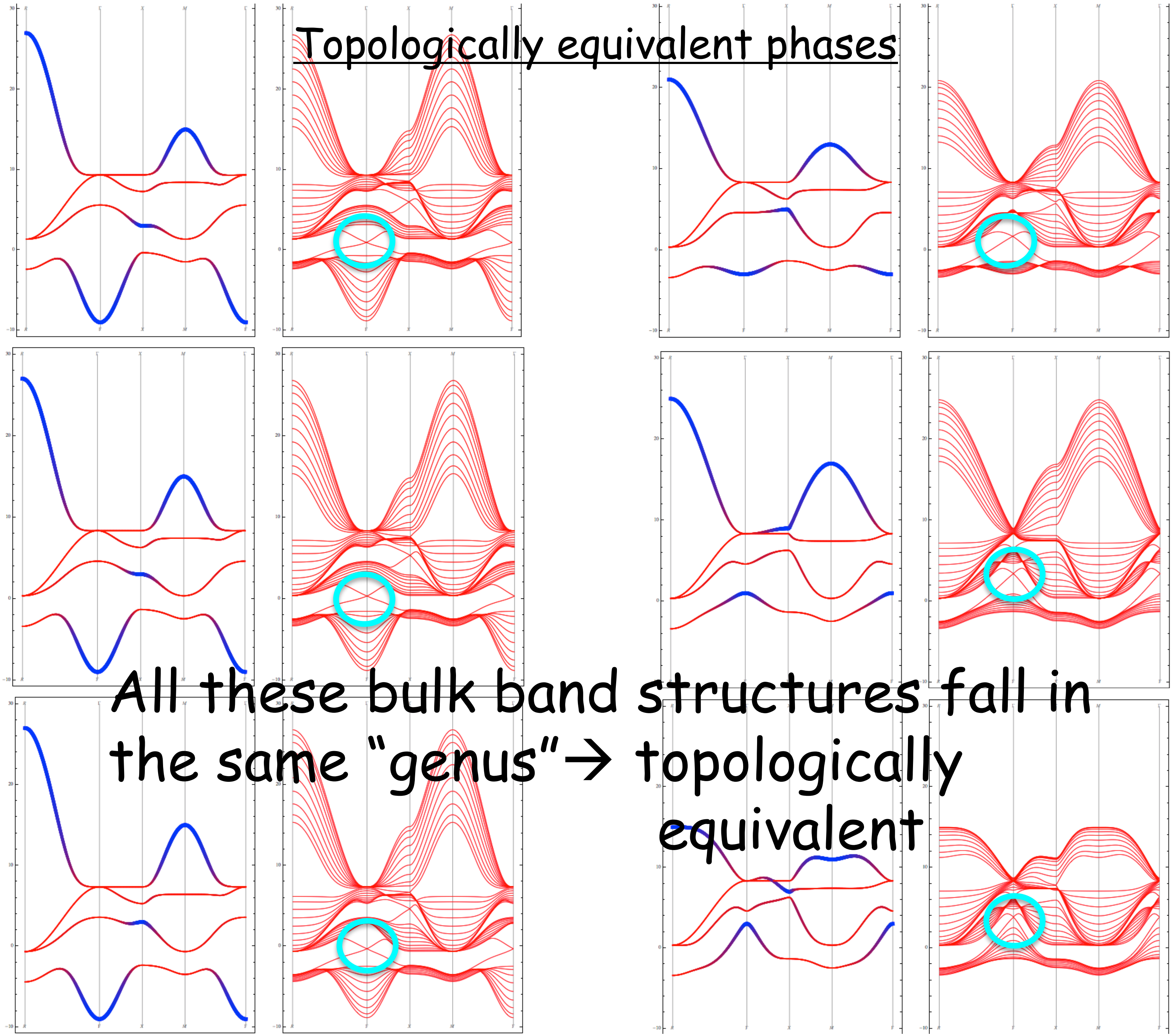


## Topologically equivalent phases



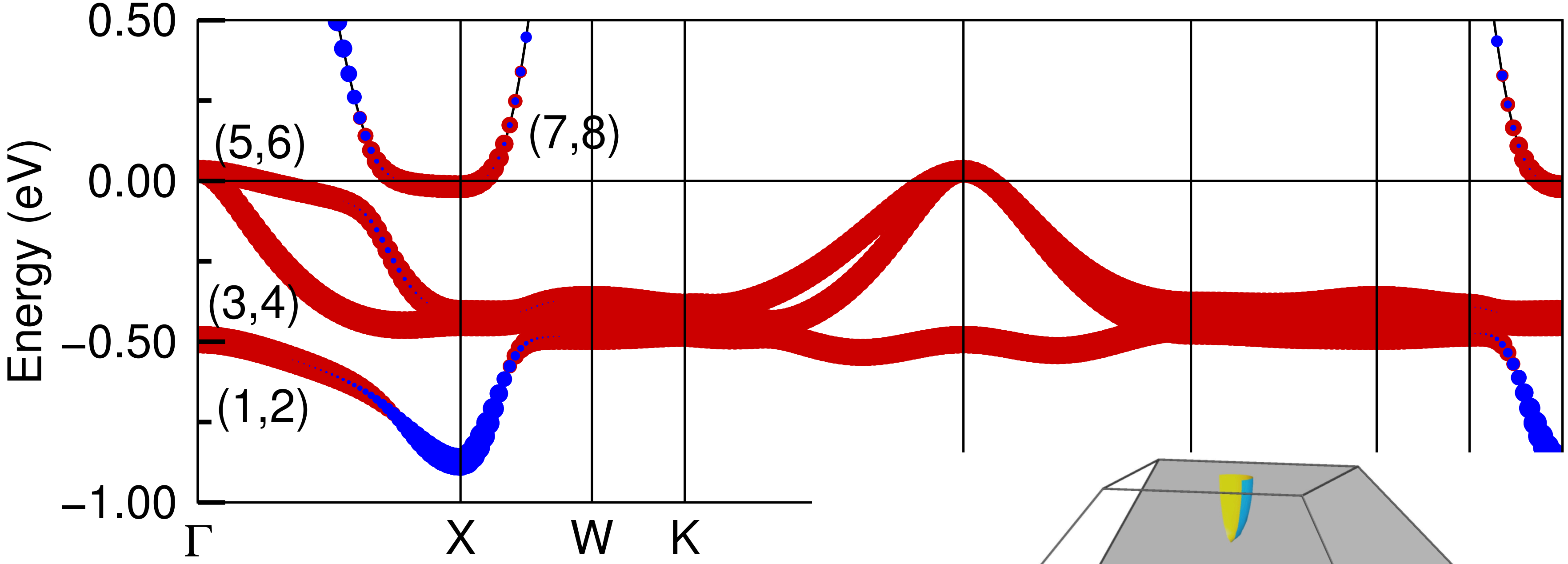
All these bulk band structures fall in the same “genus”→ topologically equivalent

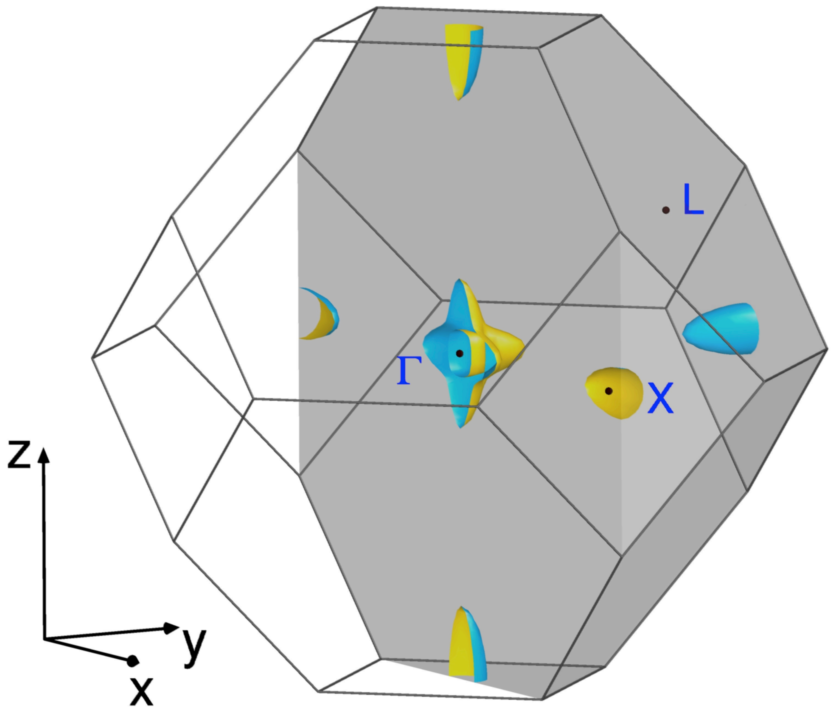
# Topologically equivalent phases

Is there an example in real condensed matter, where many different topologically equivalent phases can be found ?

Example : SmO

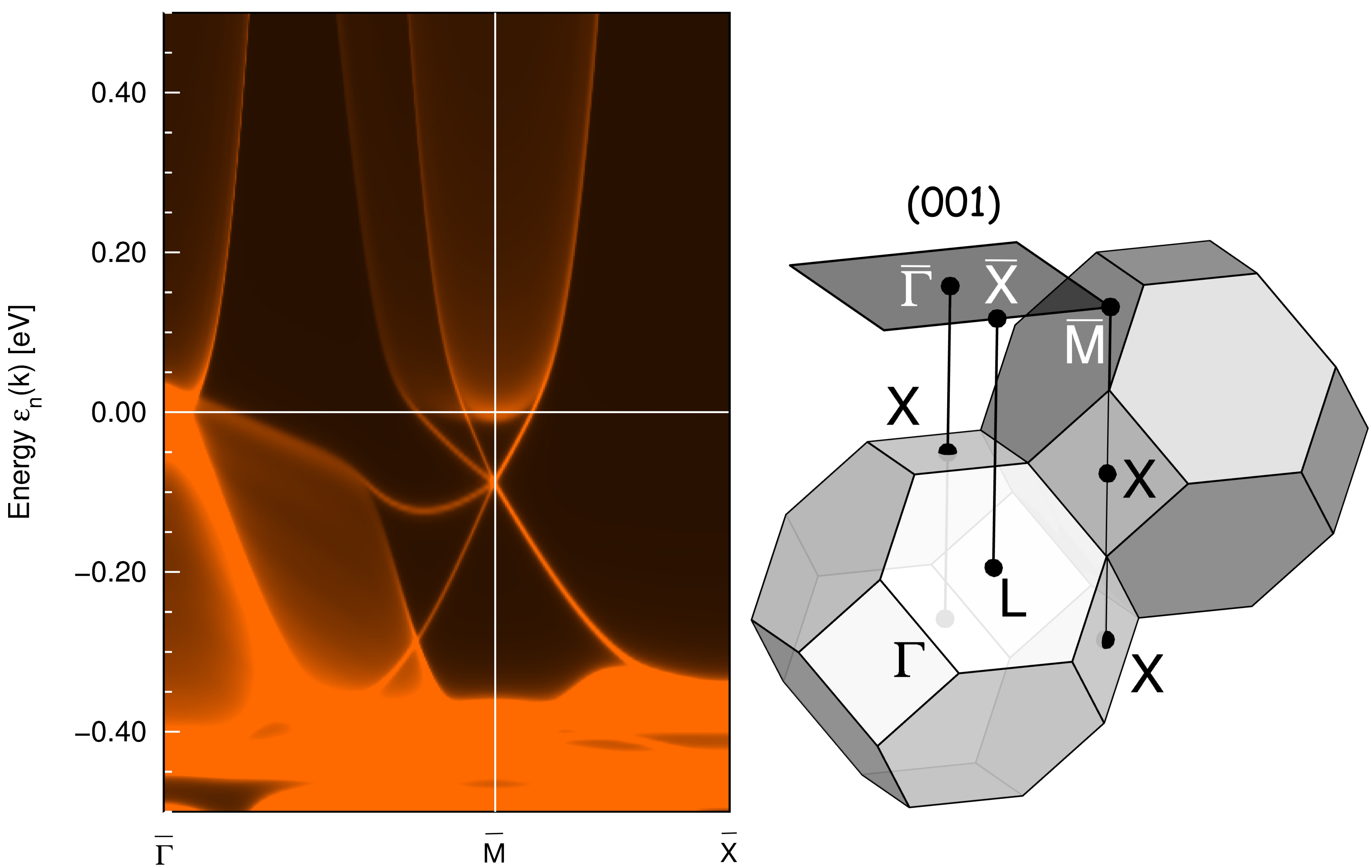
# SmO: band structure

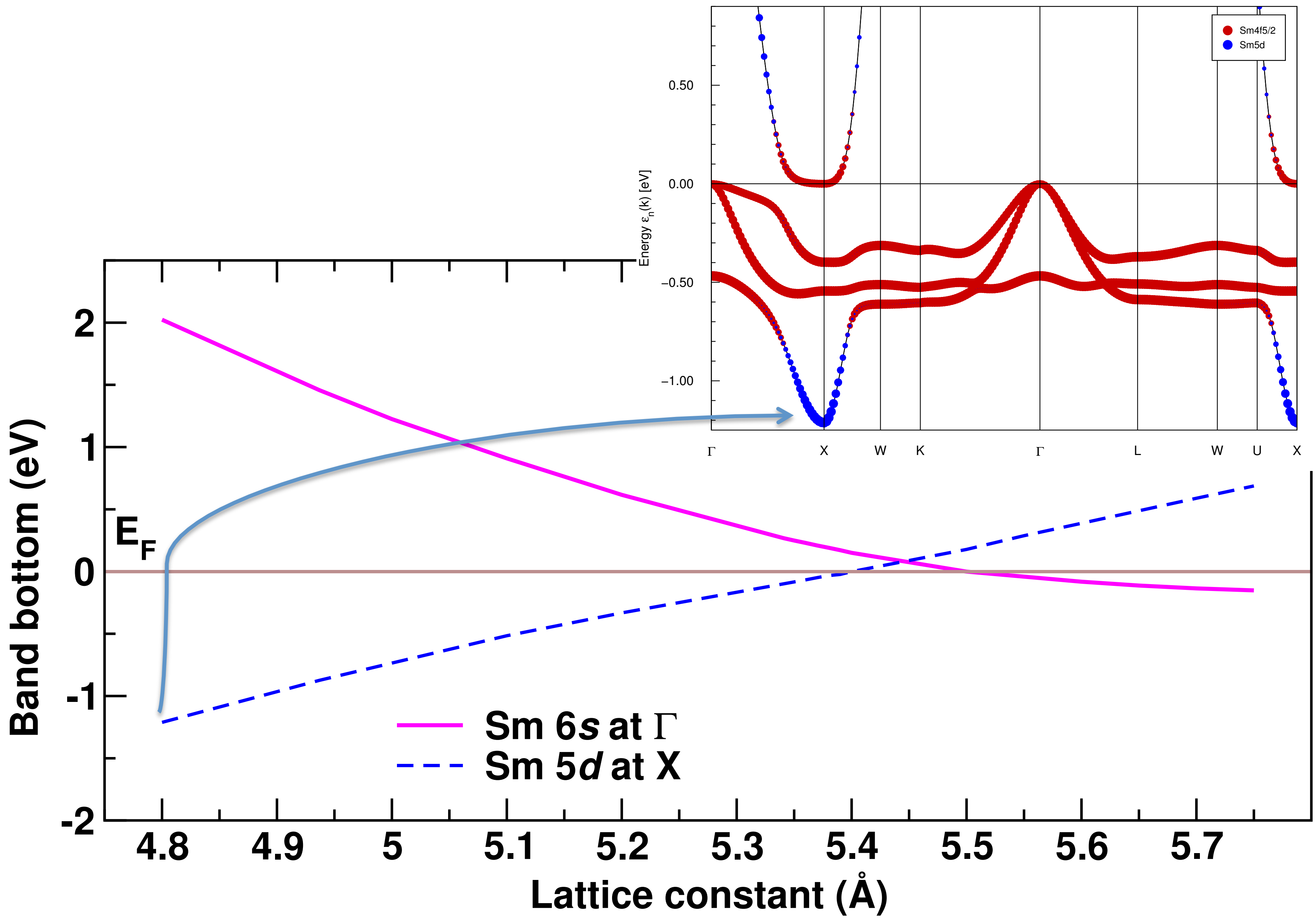


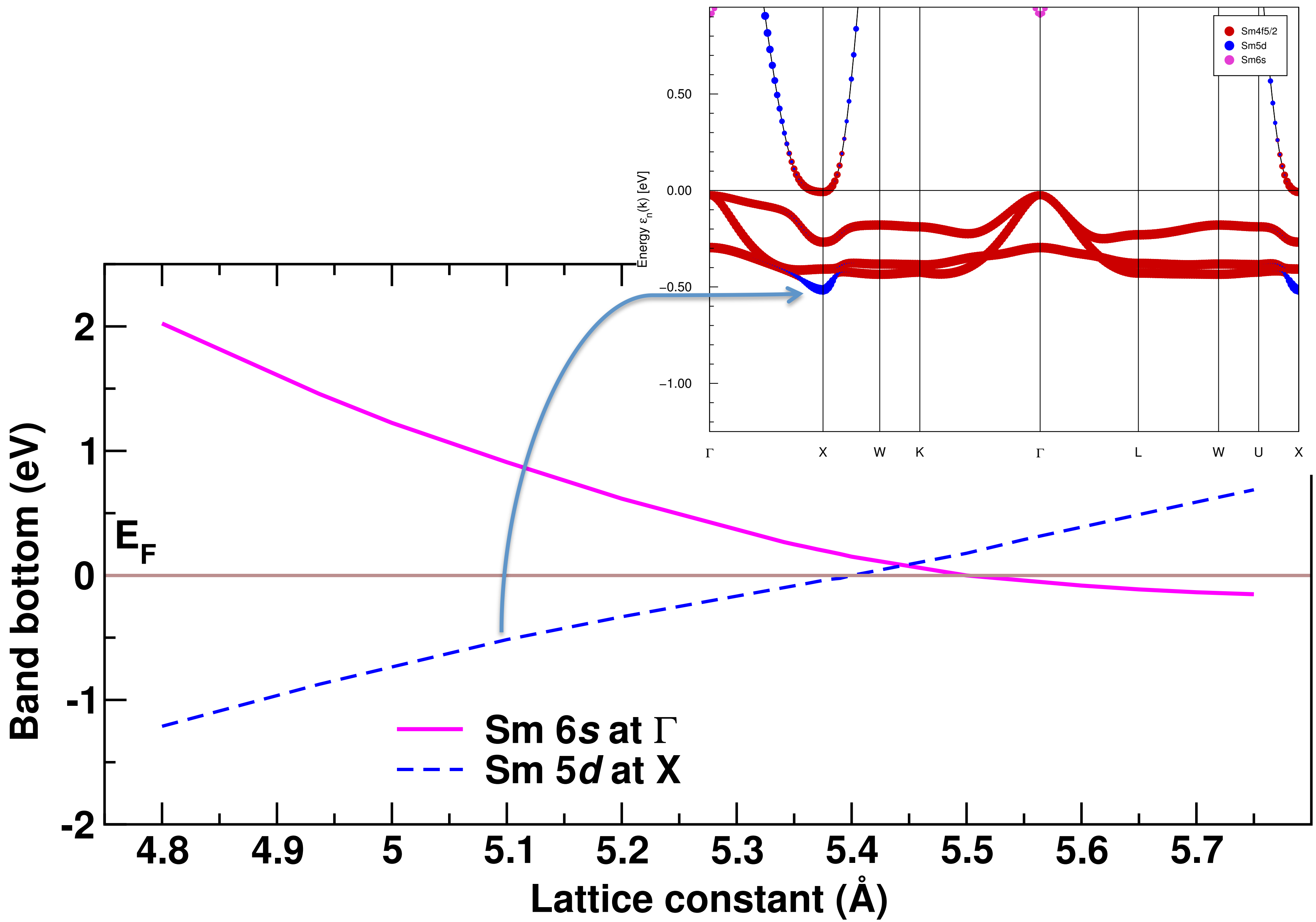

SmO is a semi-metal with a "warped" band gap

# SmO (001) surface

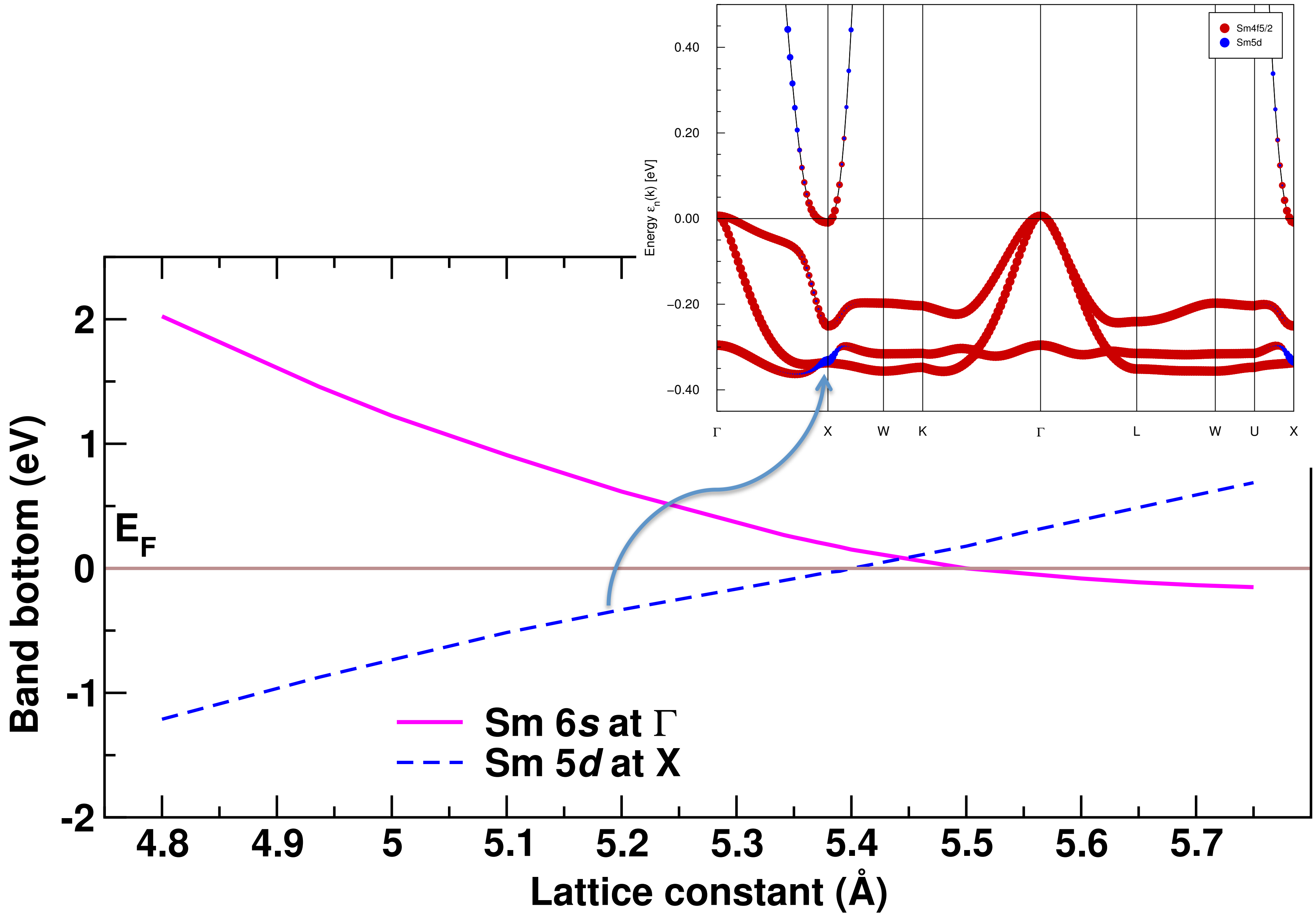




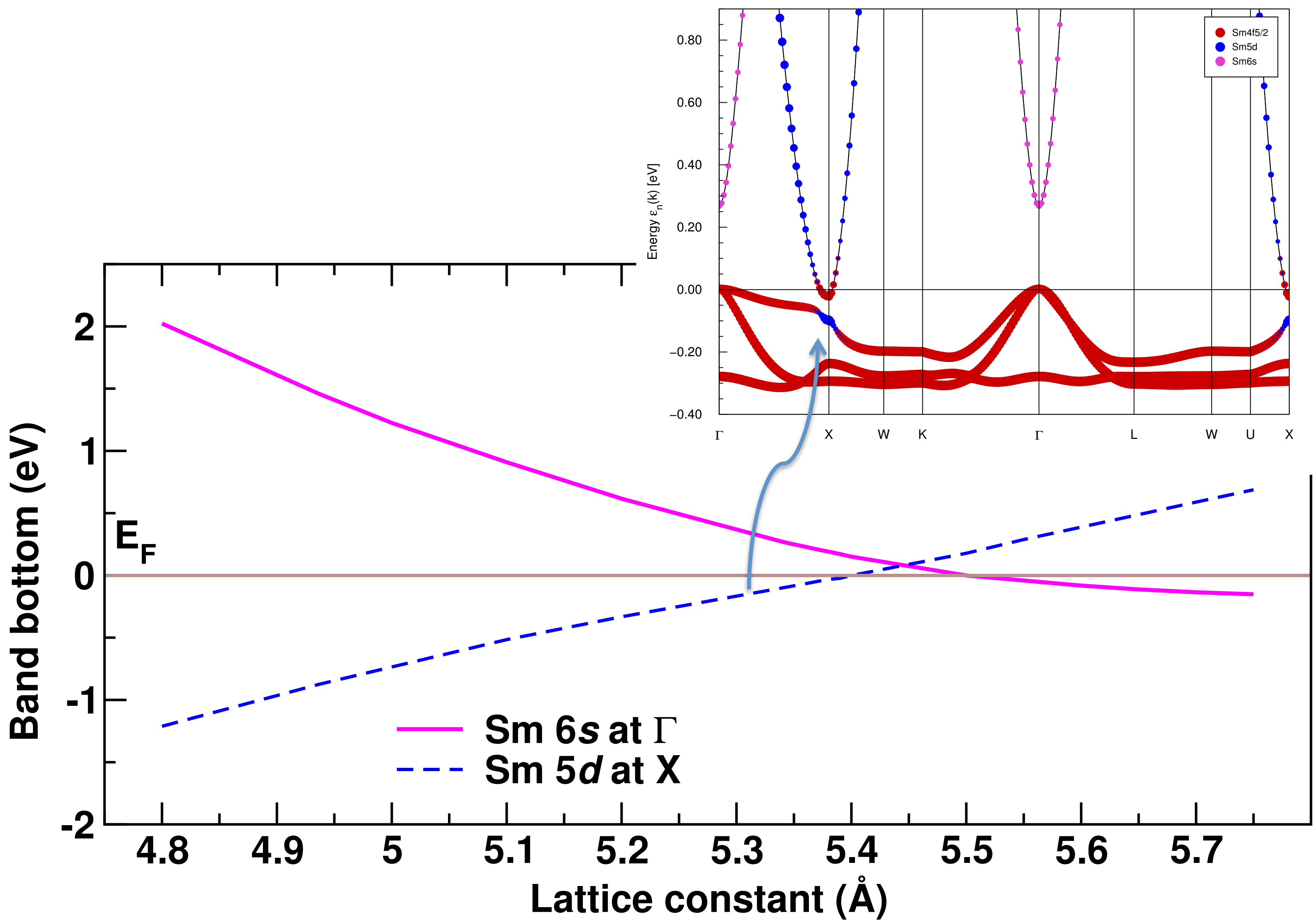
Band bottom (eV)
Lattice constant (Å)
E_F
Sm 6s at Γ
Sm 5d at X
Sm4f5/2
Sm5d
Energy ε_n(k) [eV]
Γ X W K Γ L W U X



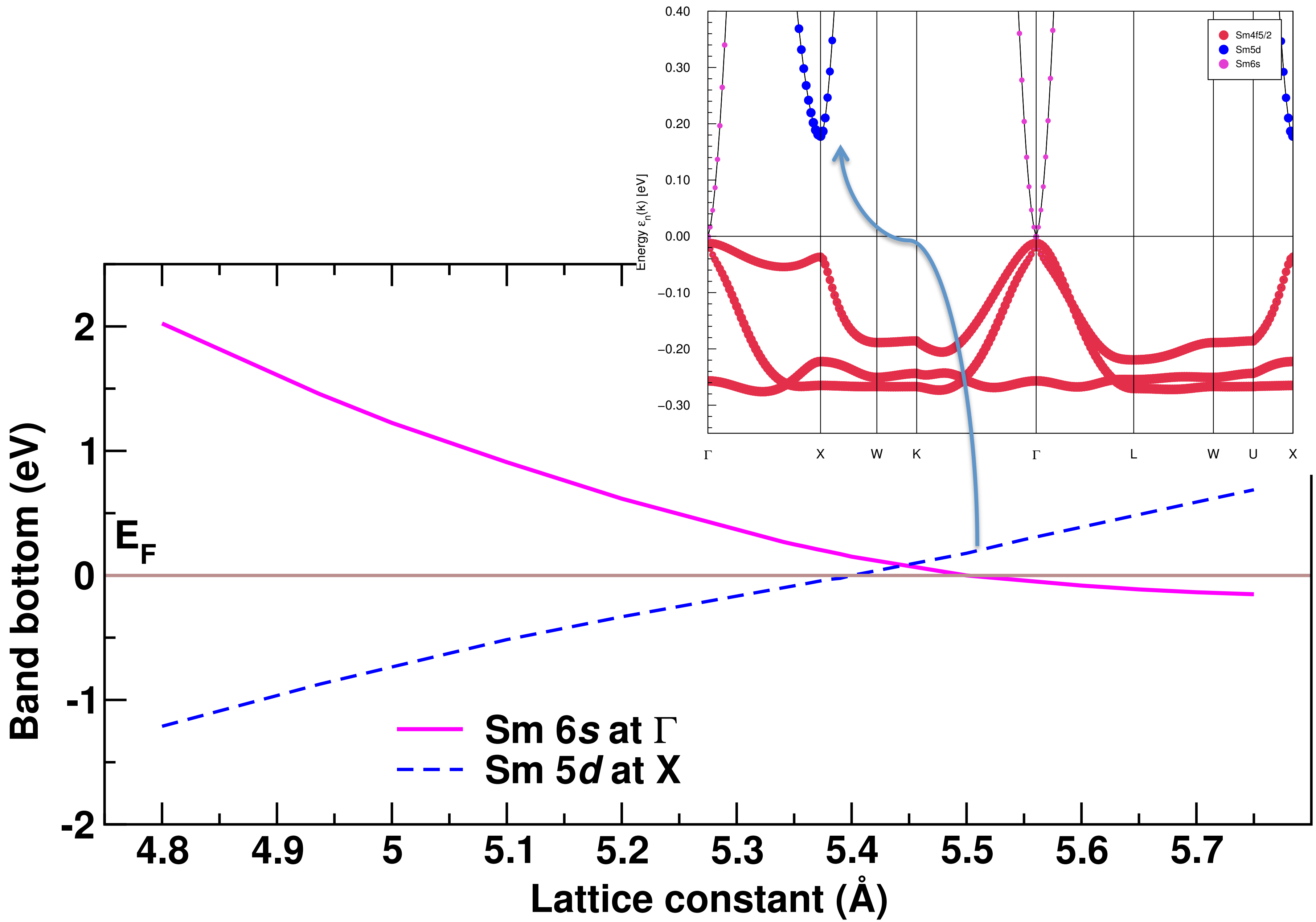
Band bottom (eV)
Lattice constant (Å)
E$_F$
Sm 6$s$ at Γ
Sm 5$d$ at X
2
1
0
-1
-2
4.8
4.9
5
5.1
5.2
5.3
5.4
5.5
5.6
5.7
Energy $\varepsilon_n(k)$ [eV]
0.50
0.00
−0.50
−1.00
Γ
X
W
K
Γ
L
W
U
X
Sm4f5/2
Sm5d
Sm6s



Band bottom (eV)
Lattice constant (Å)
E_F
Sm 6s at Γ
Sm 5d at X
2
1
0
-1
-2
4.8
4.9
5
5.1
5.2
5.3
5.4
5.5
5.6
5.7
Energy ε_n(k) [eV]
Sm4f5/2
Sm5d
0.40
0.20
0.00
−0.20
−0.40
Γ
X
W
K
Γ
L
W
U
X



Band bottom (eV)
2
1
0
-1
-2
E_F
4.8
4.9
5
5.1
5.2
5.3
5.4
5.5
5.6
5.7
Lattice constant (Å)
Sm 6s at Γ
Sm 5d at X
Energy ε_n(k) [eV]
0.80
0.60
0.40
0.20
0.00
−0.20
−0.40
Γ
X
W
K
Γ
L
W
U
X
Sm4f5/2
Sm5d
Sm6s



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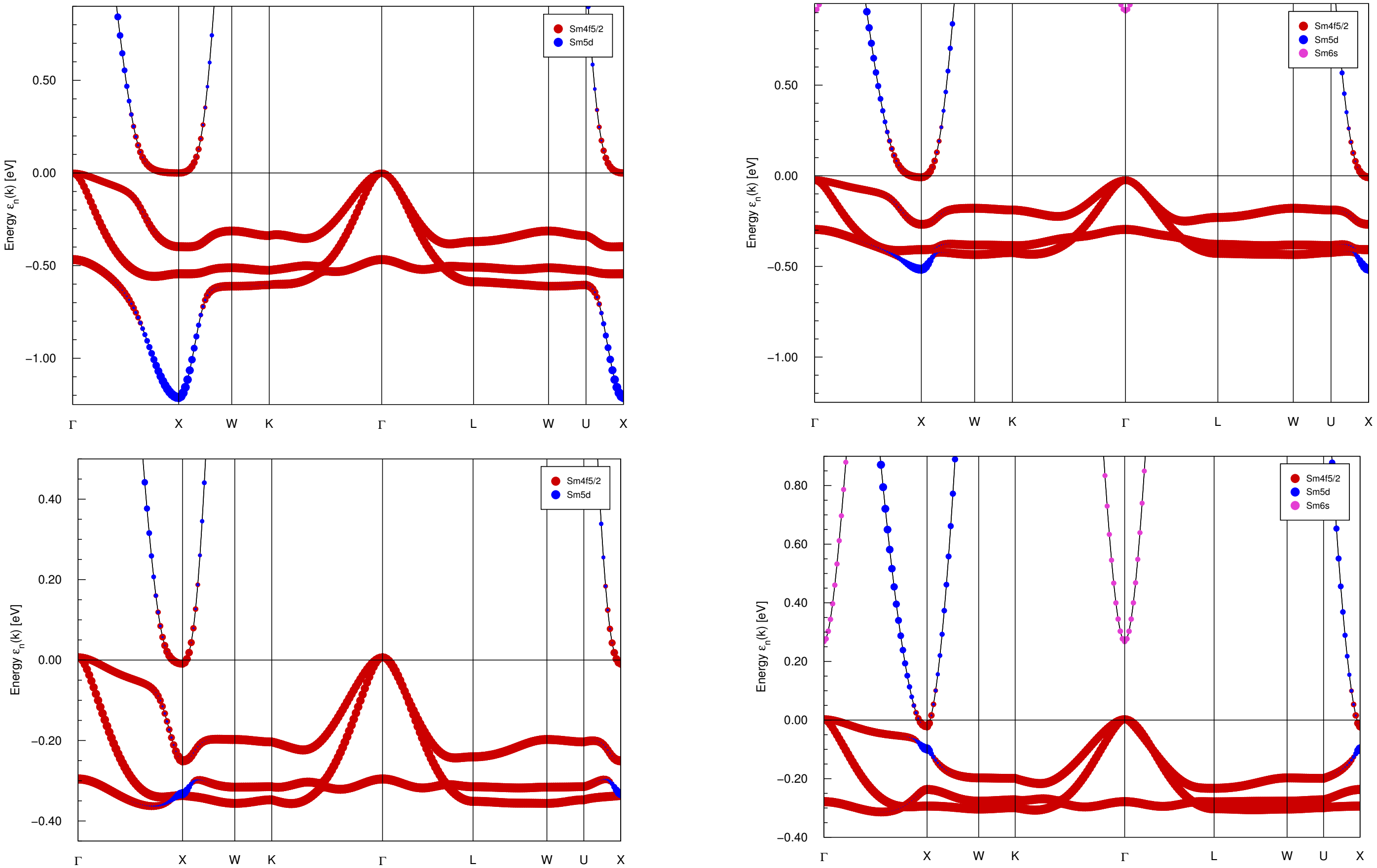
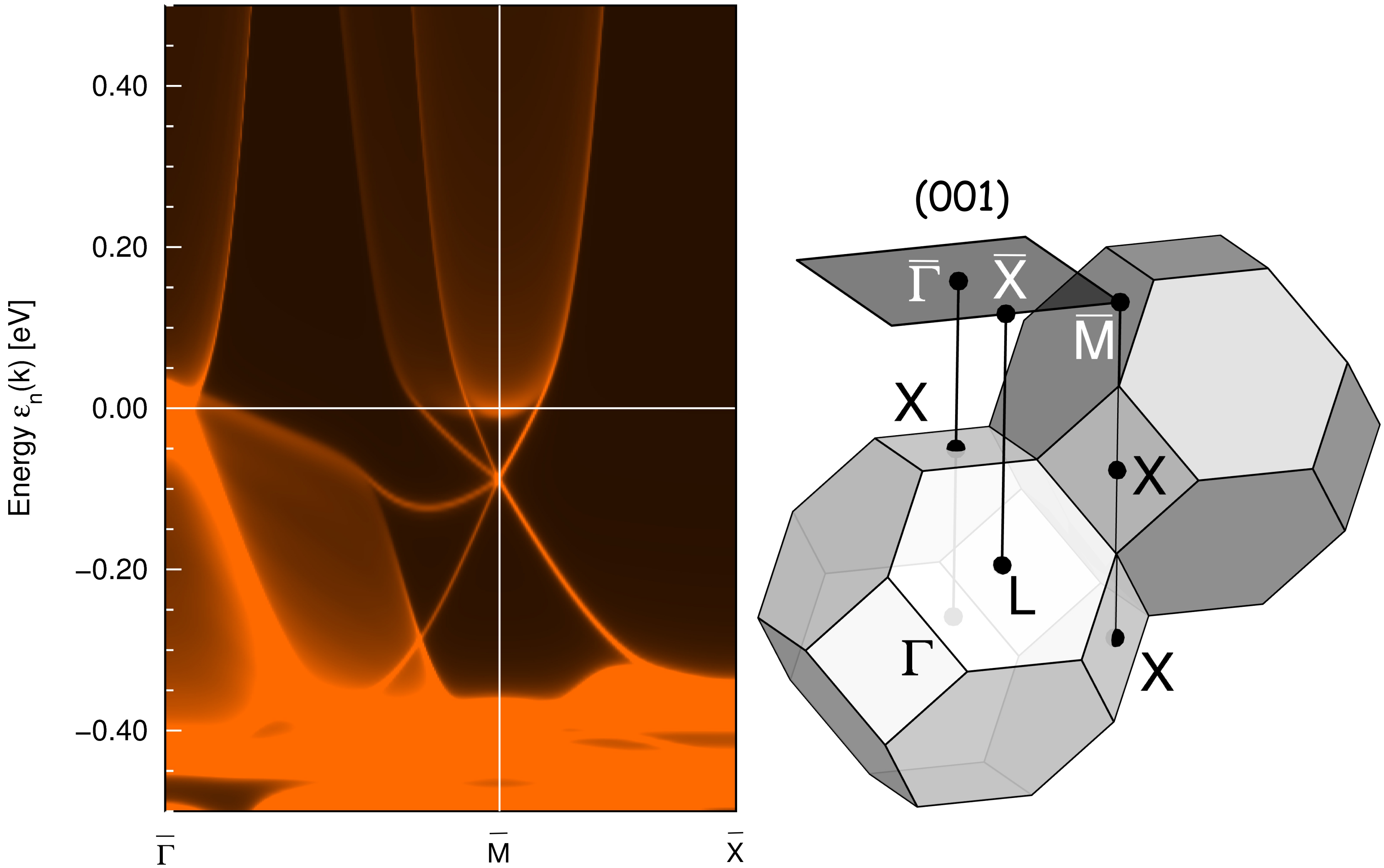
Lattice constant (Å)
$E_F$
Sm 6*s* at Γ
Sm 5*d* at X
Energy $\varepsilon_n(k)$ [eV]
Sm4f5/2
Sm5d
Sm6s
Γ X W K Γ L W U X




Band gap never closed, even though the band structure changes a lot → all these band structures of SmO are topologically equivalent (same genus)

# SmO (001) surface



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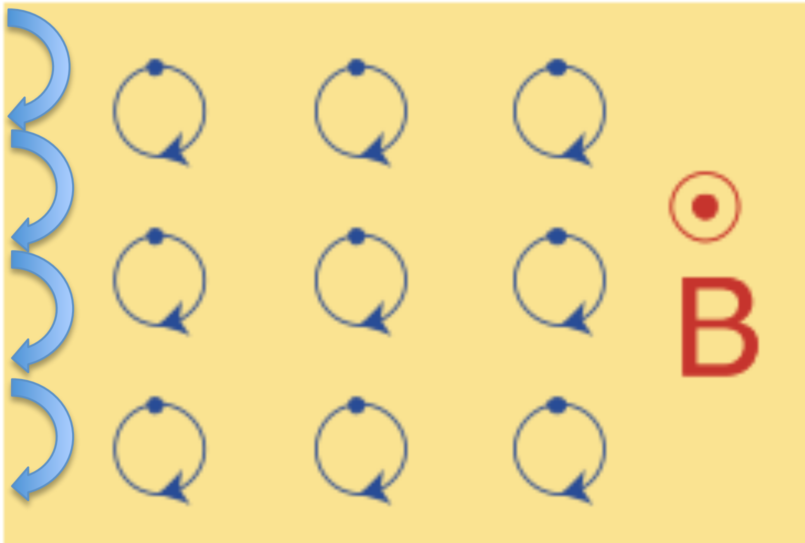


Application of magnetic field → breaks "Time Reversal Symmetry" → creation of conducting edge states.

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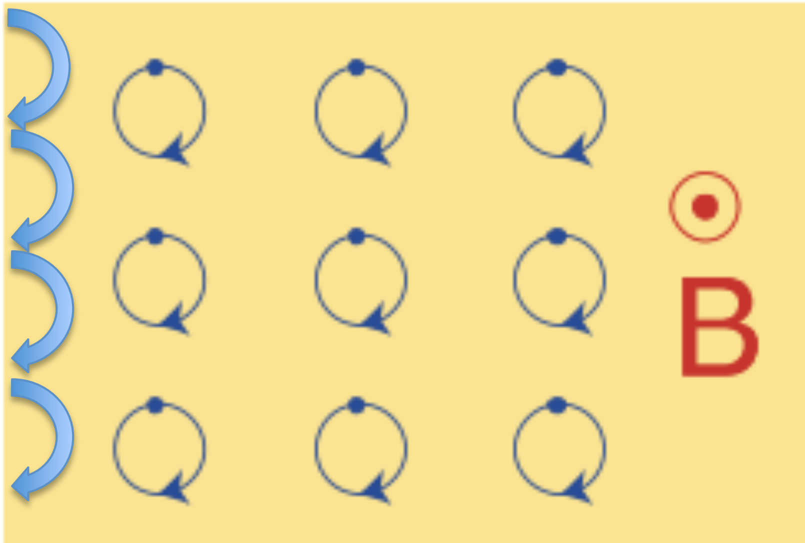


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It was assumed therefore, special edge states only occur when "time reversal symmetry" is broken.

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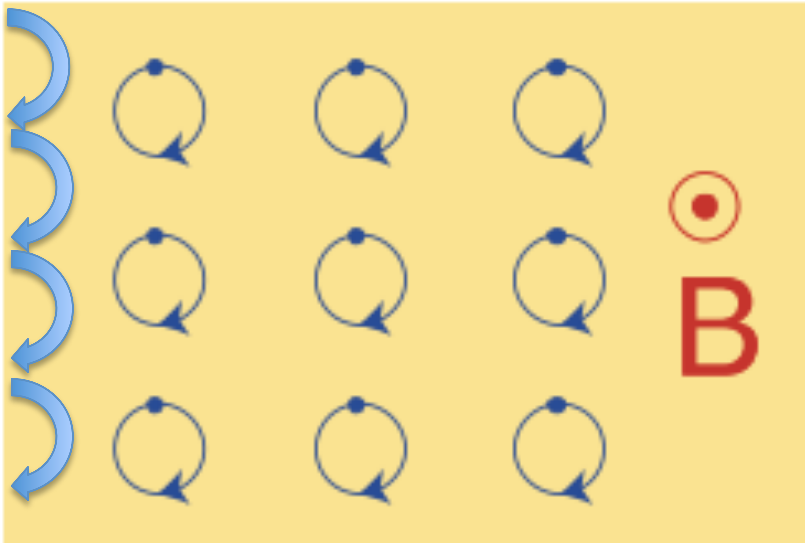


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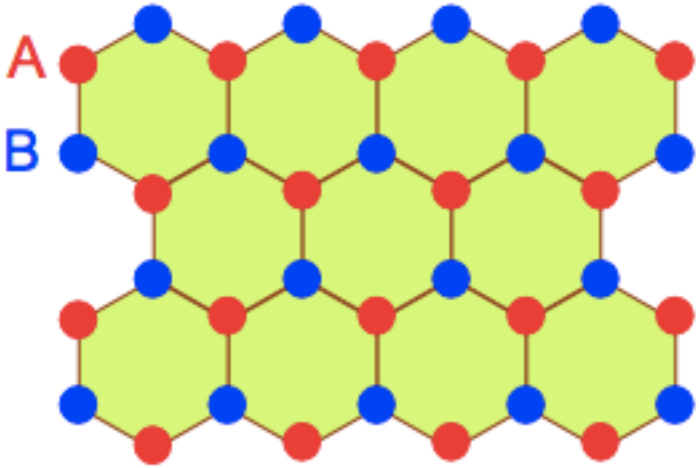
But, in band theory, which has both "time reversal" and "inversion" → one can still get edge states → example of Graphene

# Graphene




Graphene is an allotrope of carbon, which form two-dimensional hexagonal lattice.

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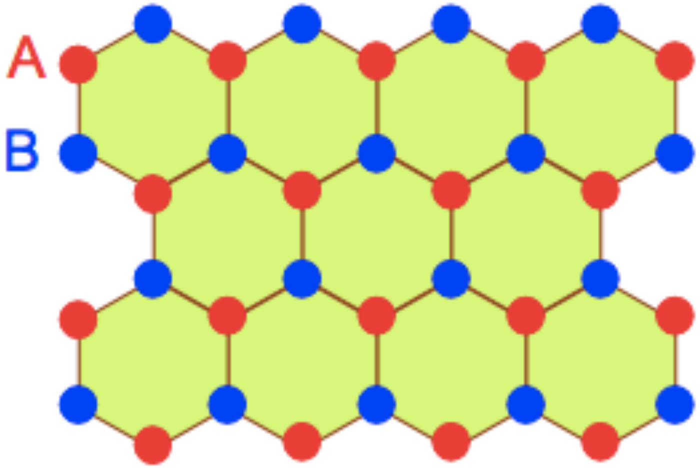
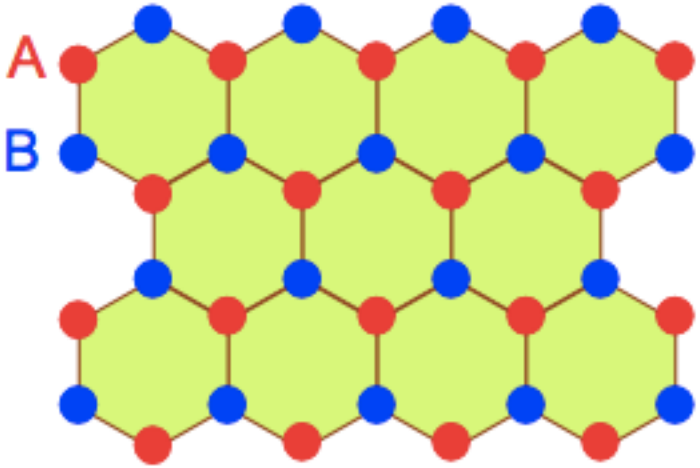



Graphene is an allotrope of carbon, which form two-dimensional hexagonal lattice.

When doing band structure calculations → requires periodic boundary conditions → we stack up these two-dimensional sheets far apart from each other, so we are essentially only capturing the physics in the sheets.

# Graphene

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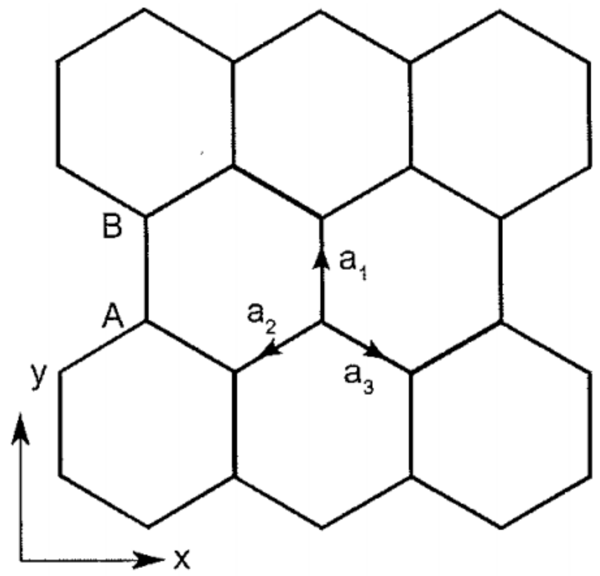
Time reversal symmetry → $d_z(k) = d_z(-k)$
Inversion symmetry → $d_z(k) = -d_z(-k)$

# Graphene

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Time reversal symmetry → $d_z(k) = d_z(-k)$
Inversion symmetry → $d_z(k) = -d_z(-k)$

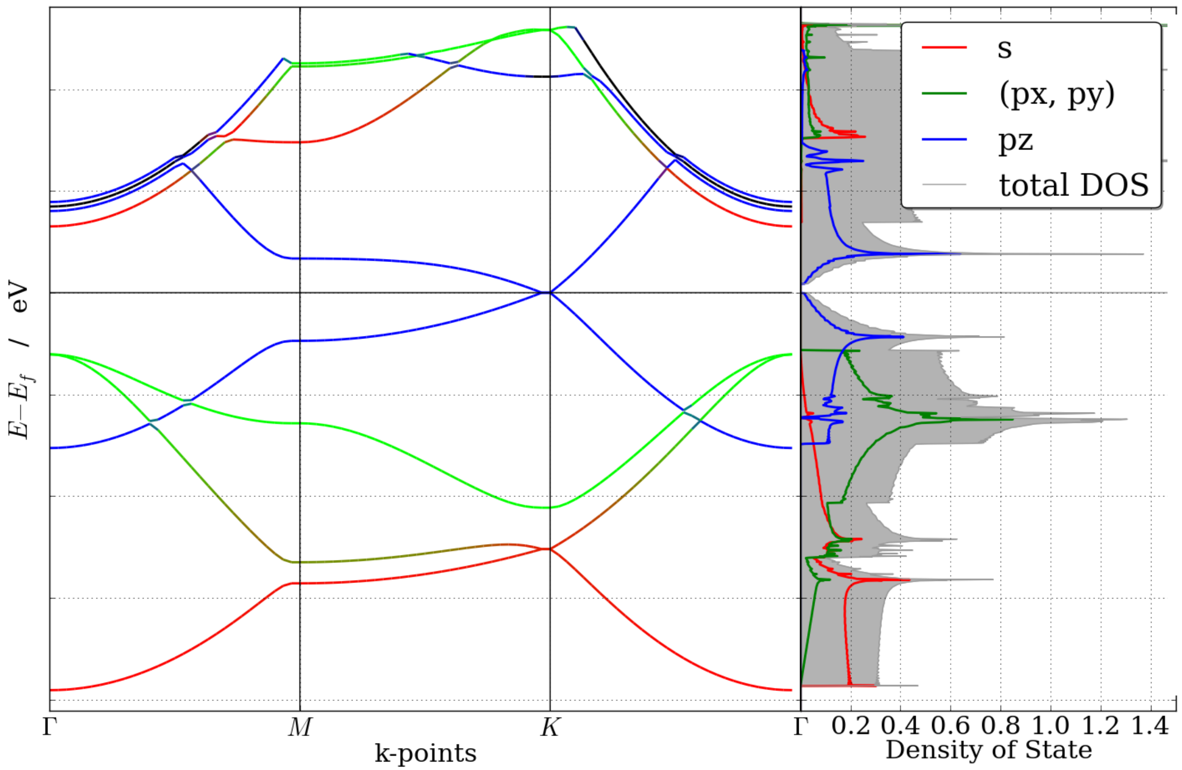
Therefore, Hamiltonian can be written as:

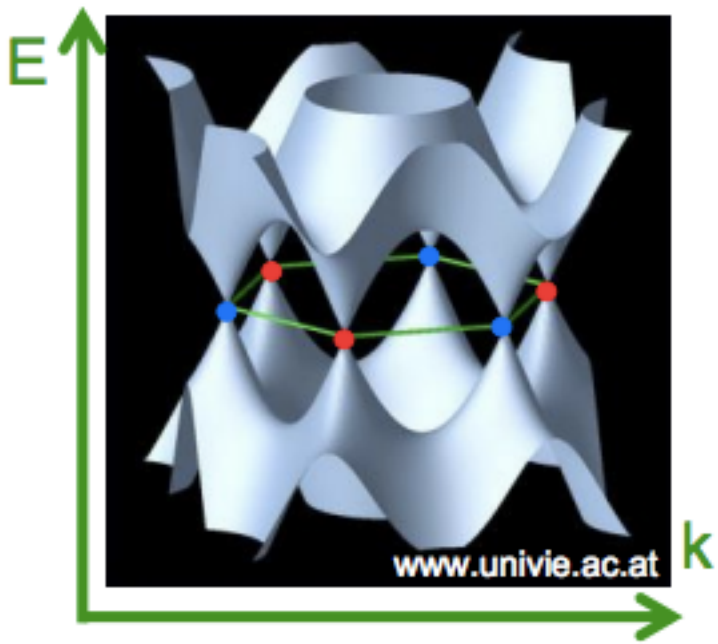
$$d_x(\mathbf{k}) = -t \sum_{p=1}^{3} \cos \mathbf{k} \cdot \mathbf{a}_p,$$

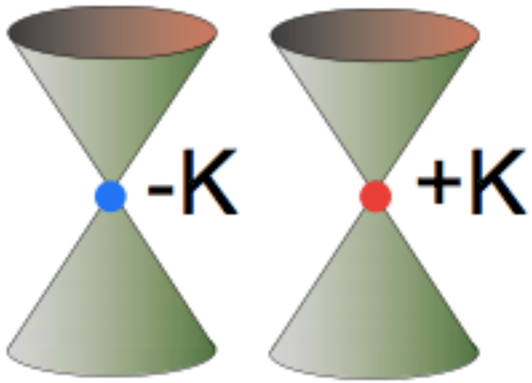
$$d_y(\mathbf{k}) = -t \sum_{p=1}^{3} \sin \mathbf{k} \cdot \mathbf{a}_p,$$

$$d_z(\mathbf{k}) = 0.$$

# Graphene




Point zeroes in ($d_x$, $d_y$) due to inversion and time reversal symmetry