Julius-Maximilians-UNIVERSITÄT WÜRZBURG

AG Sangiovanni

Engineering correlated orbitals: metal-insulator and topological phase transitions

In collaboration with

- Severino Adler
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- Alessandro Toschi
  Karsten Held (Vienna)
- Tim Wehling (Bremen)
  Roser Valentí (Frankfurt)
- Adriano Amaricci
  Massimo Capone (Trieste)
- Jan Budich (Dresden)
  Björn Trauzettel (Würzburg)

Dresden Würzburg
ct.qmat

Aspen (virtually), March 11. 2020

SFB 1170
physics with a twist

ToCoTronics

References: PRB **88**, 195116 (2013) — PRL **114**, 185701 (2015) — PRL **114**, 246401 (2015) — PRL **119**, 256404 (2017) — arXiv:2001.04102 (2020)

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lifting of orbital degeneracy in many-body systems

⬇

more than just renormalizing single-particle Hamiltonian parameters

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outline

- example of nickelate heterostructures (pre-d^9 nickel-age of superconductivity — H. Hwang)
- splitting of two e_g orbitals, d^7-d^8 physics

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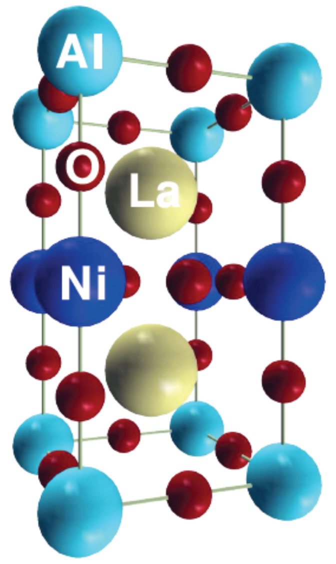

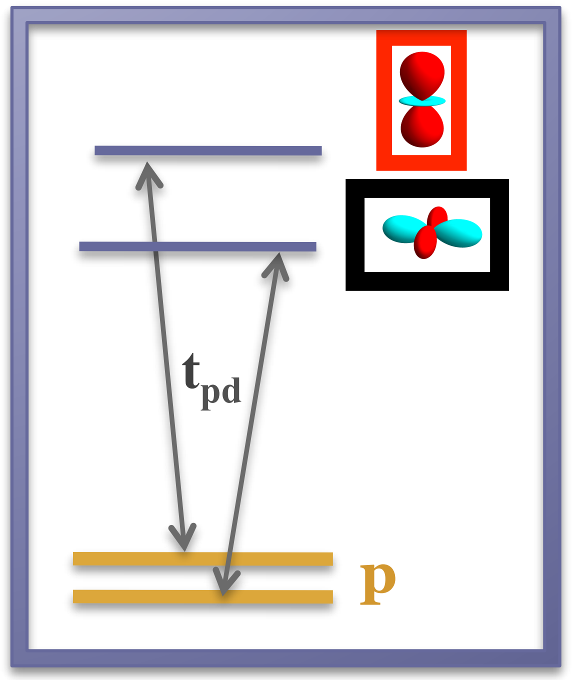

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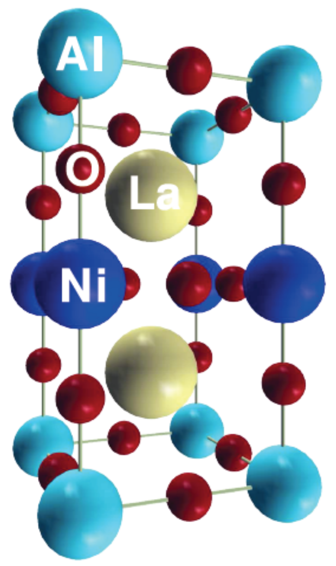
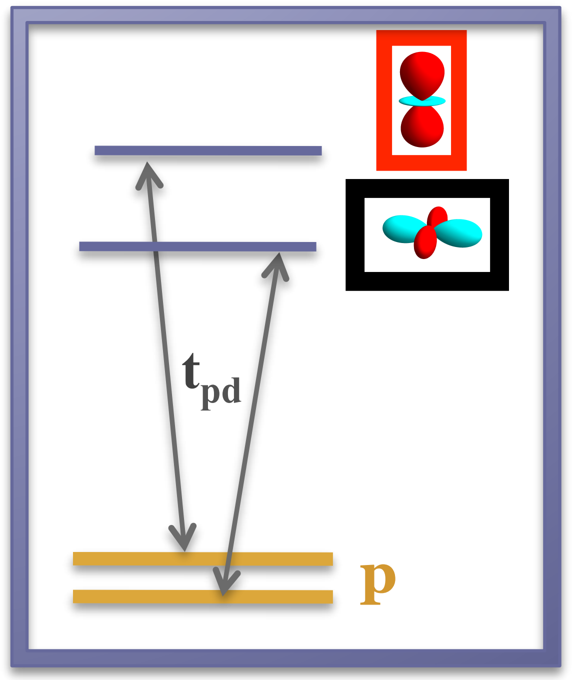
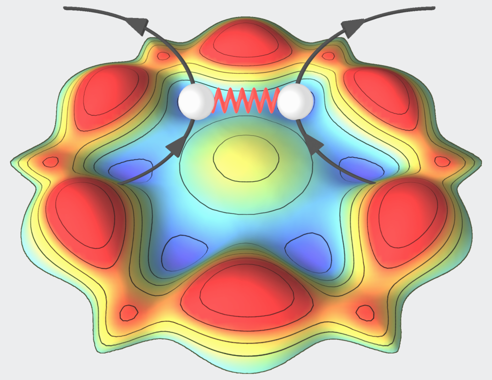




“effective” crystal-field splitting

$$\Delta_{\text{eff}}^{e_g} = \Delta_{\text{DFT}}^{e_g} + \text{Re}\Sigma_{3z^2-r^2}(\omega \to 0) - \text{Re}\Sigma_{x^2-y^2}(\omega \to 0)$$



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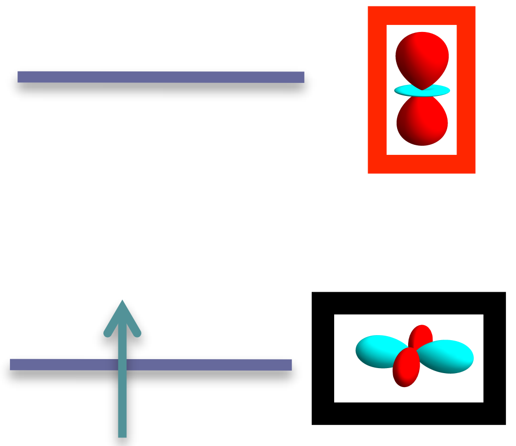

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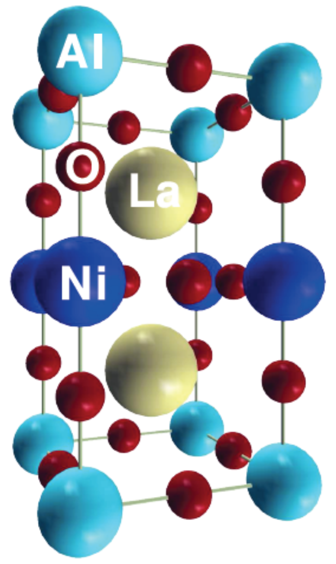

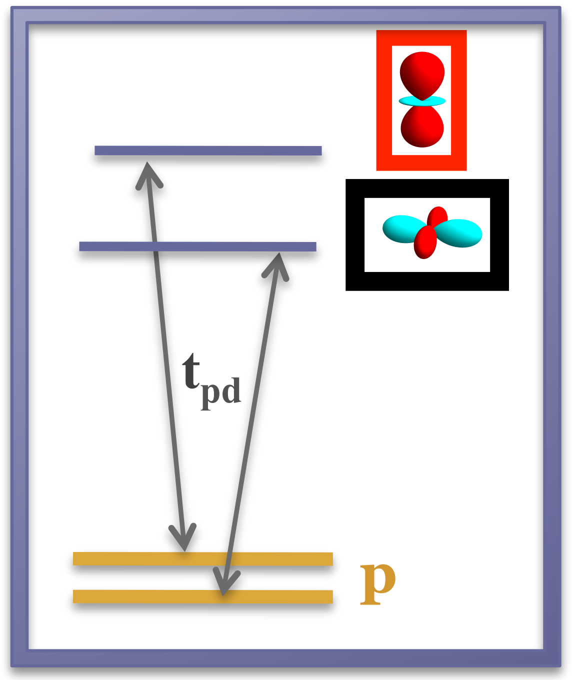

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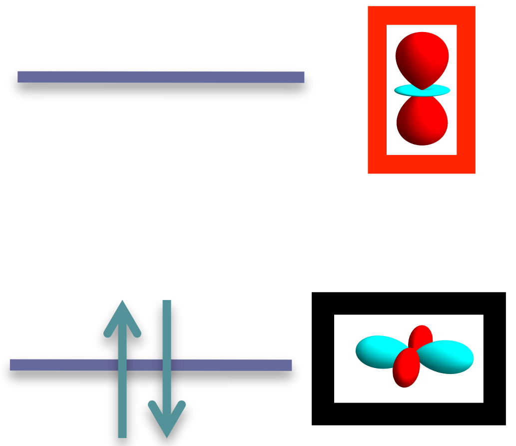

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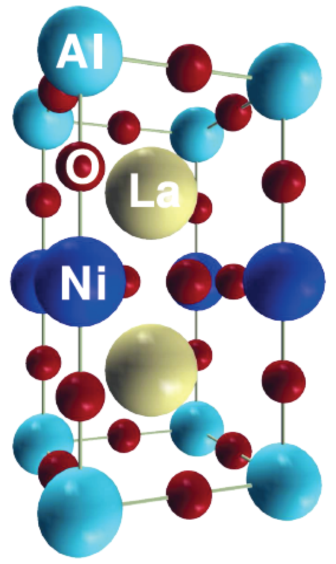

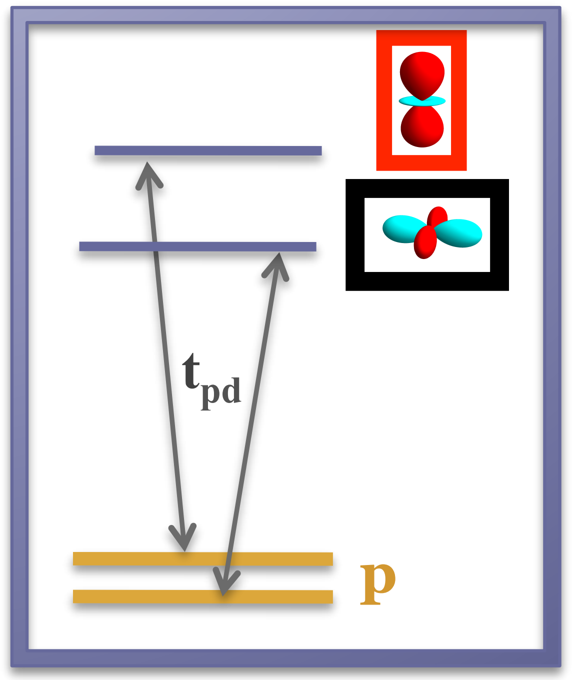

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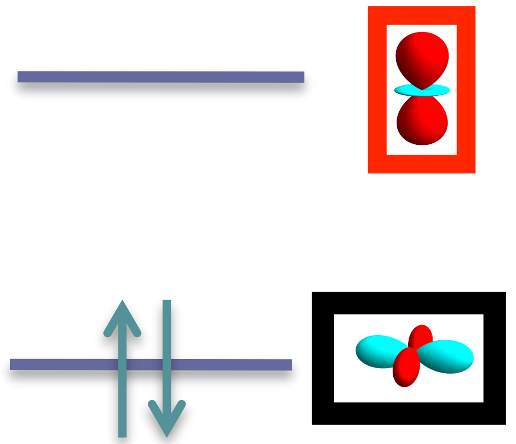

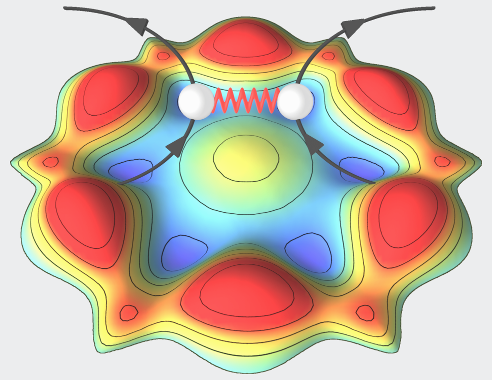

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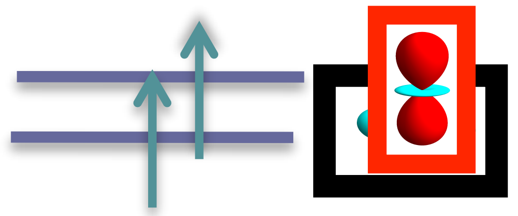

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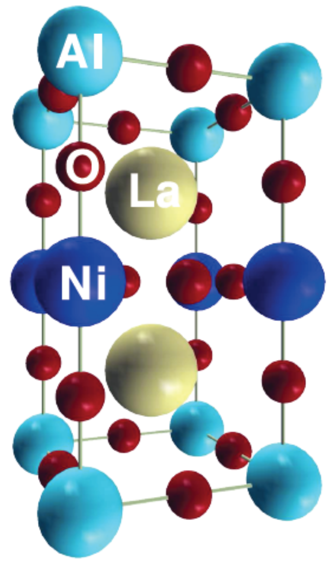

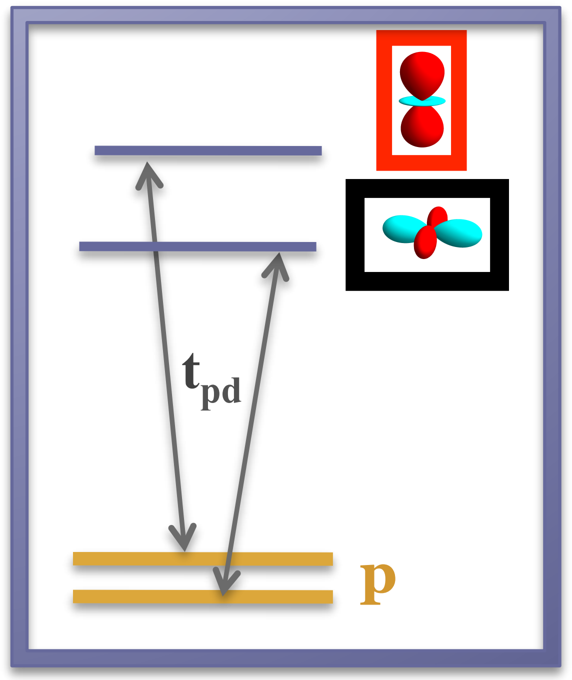

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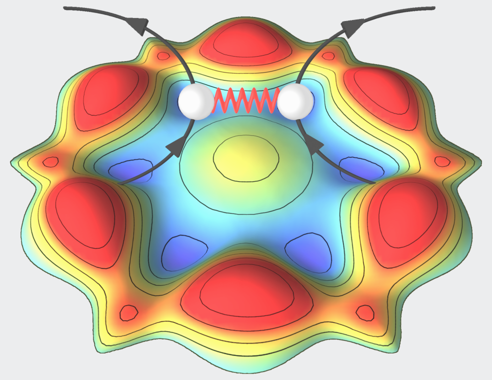

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1st part of my talk
oxide heterostructures

- inclusion of many-body effects $\Longrightarrow$ two possible results

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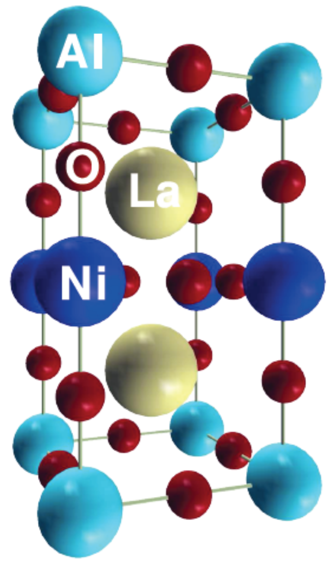
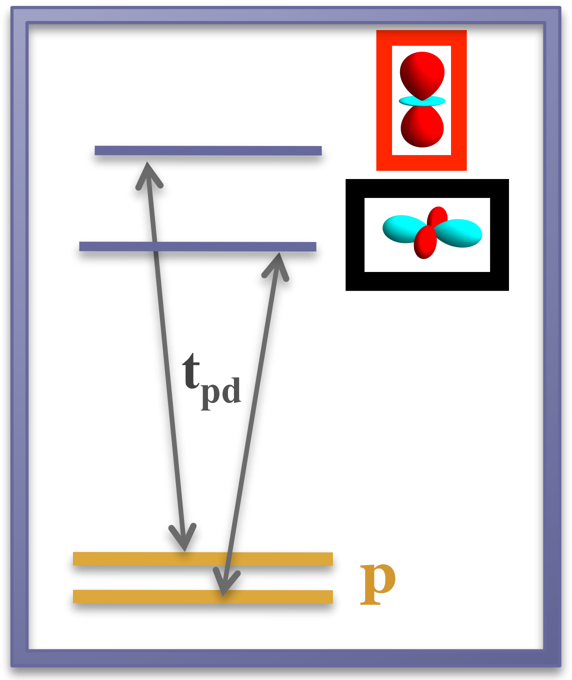
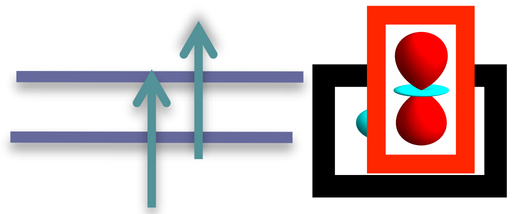




“effective” crystal-field splitting

2nd part of my talk
correlated TIs
twisted-bilayer TMD



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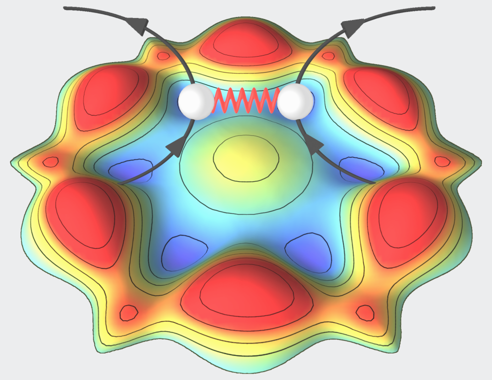

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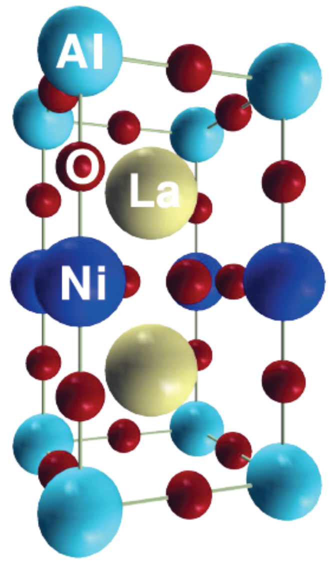

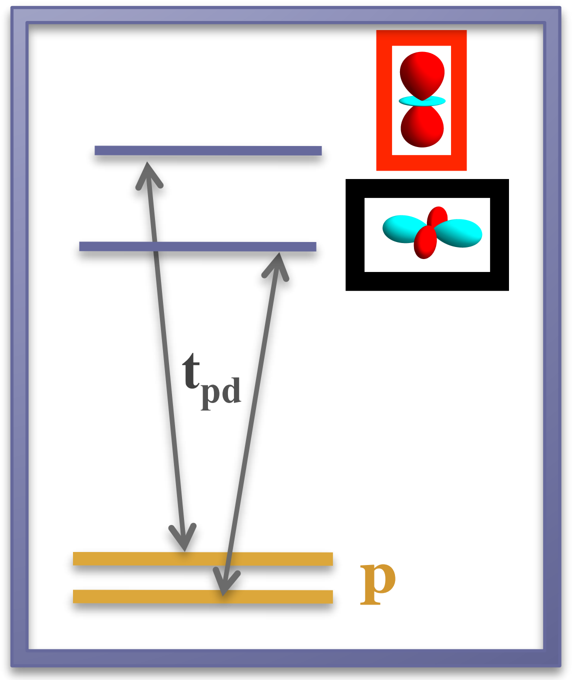

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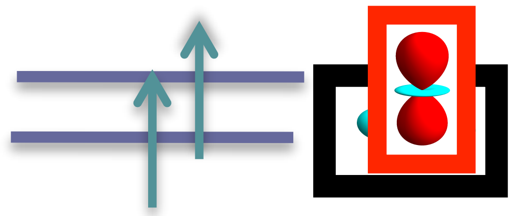

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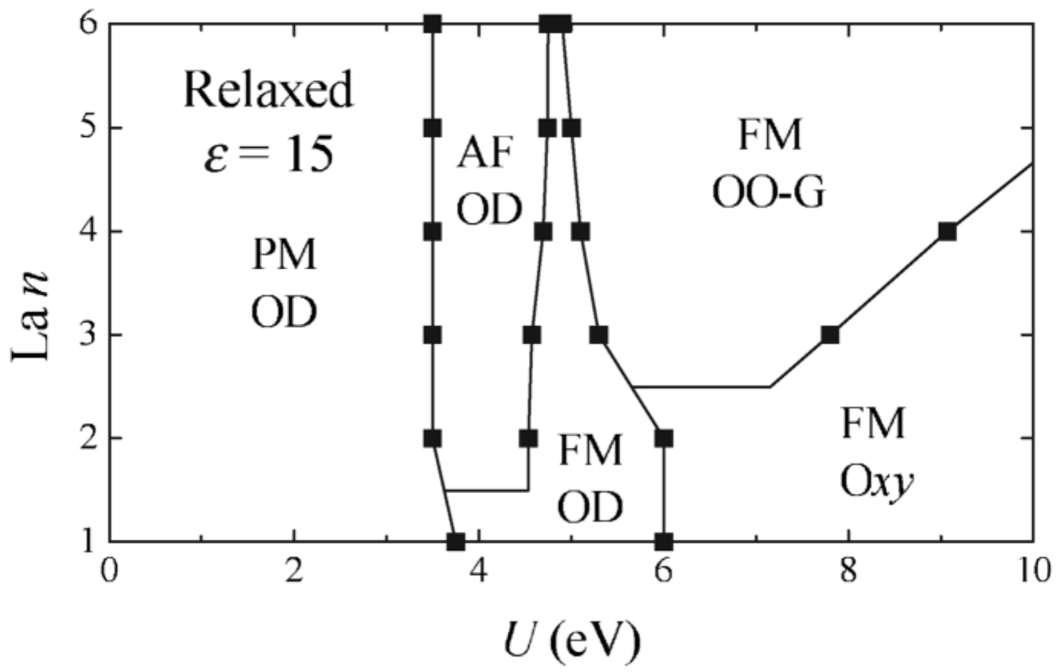
- always useful/meaningful?
- what happens when we lose such simple single-particle picture?

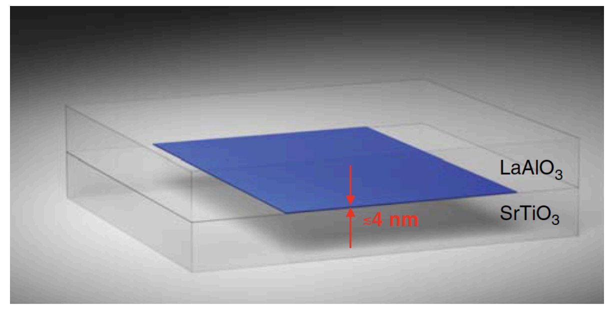
Oxide Heterostructures

- highly active field, even several years after the first pioneering contributions by H. Hwang, A. Millis, etc… [previous talk by Divine Kumah]
- platform for superconductivity and magnetism
- *d*-electrons: strong responses beyond bulk phase diagrams

LaTiO$_3$/SrTiO$_3$

Okamoto, *et al.* PRL (2006)





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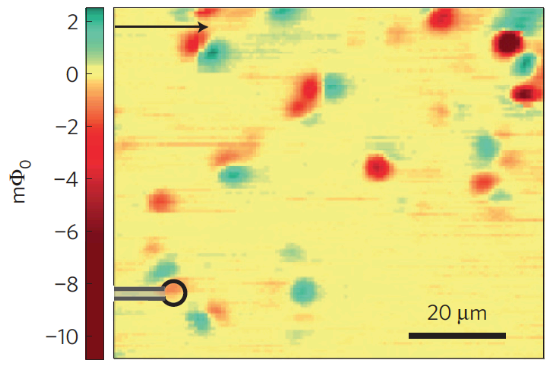

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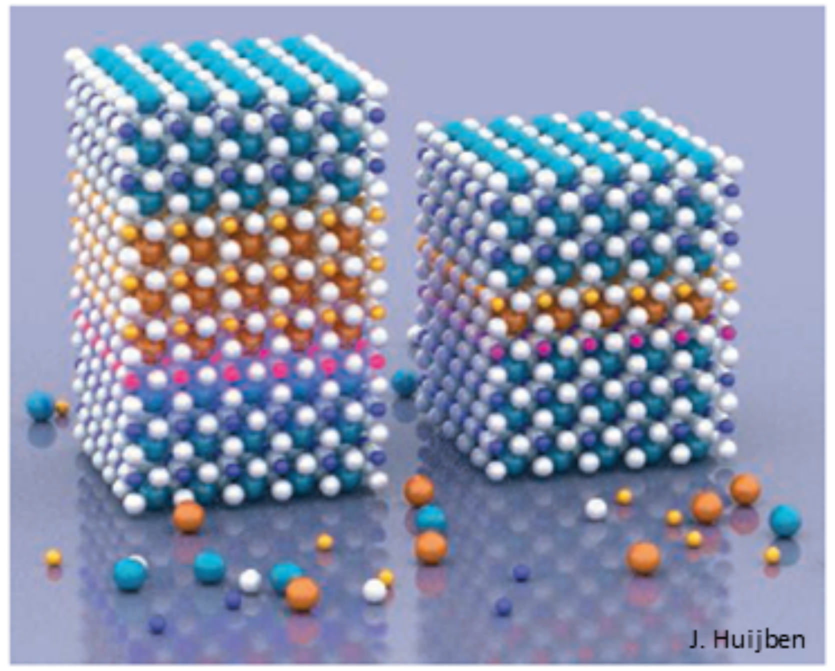

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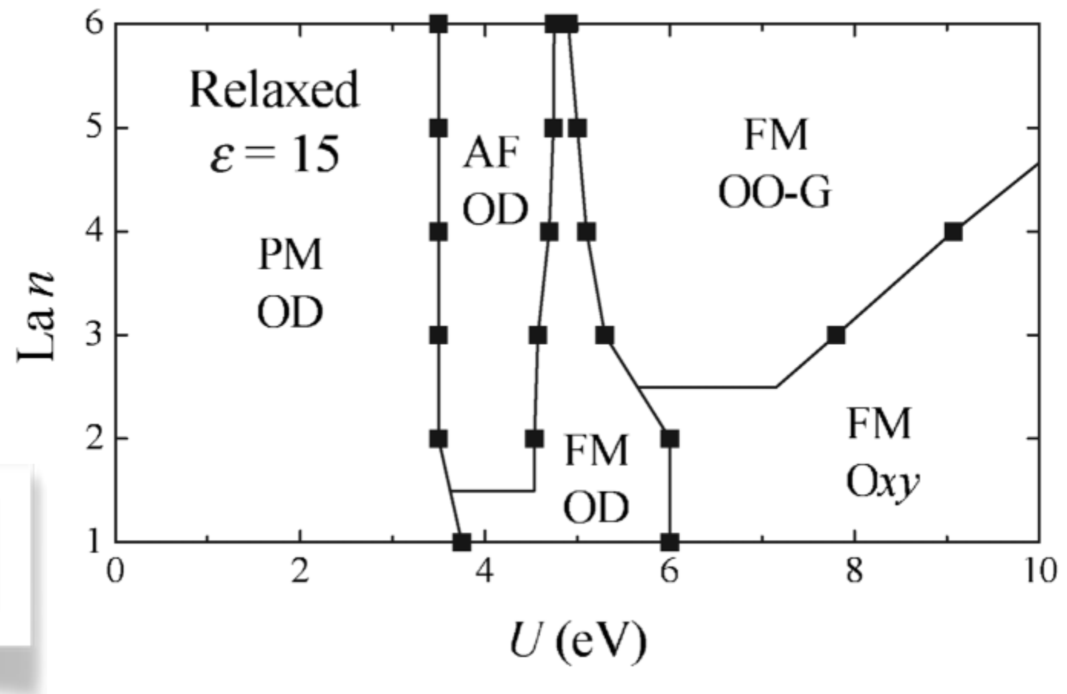
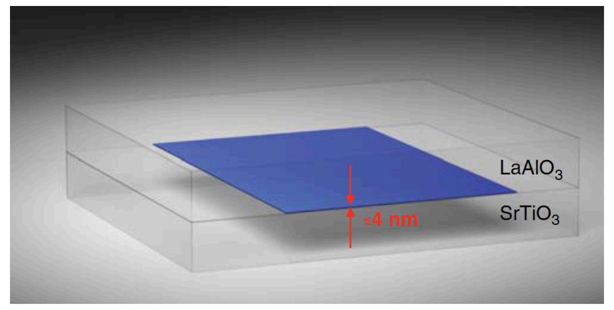
thickness-induced metal-insulator transitions





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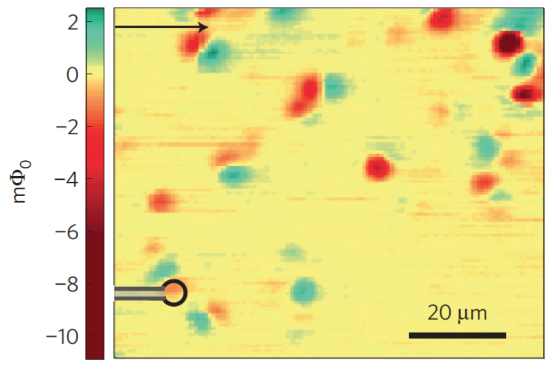

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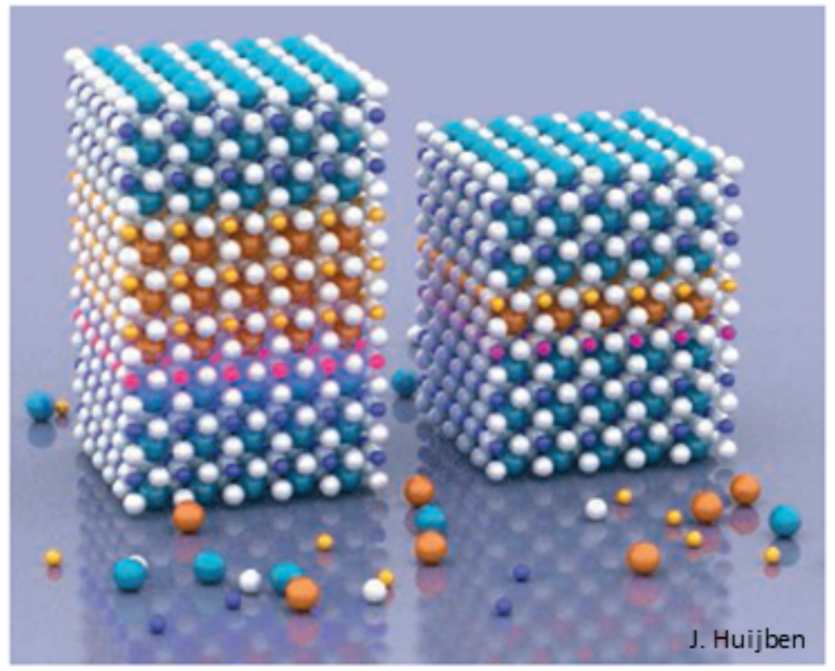

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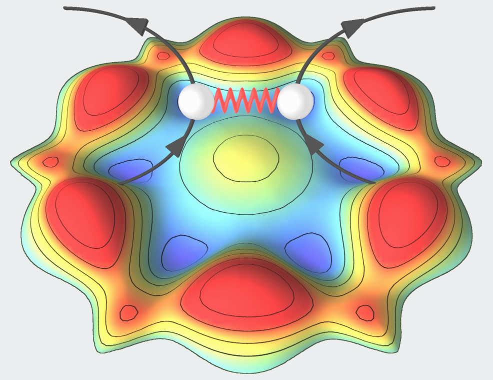

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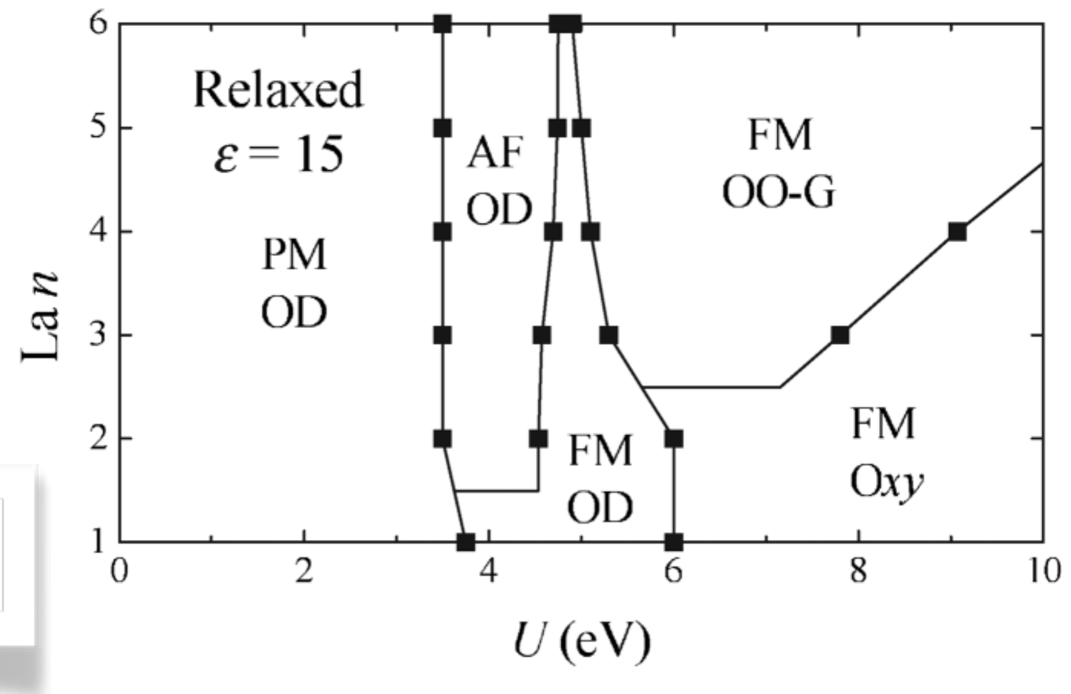

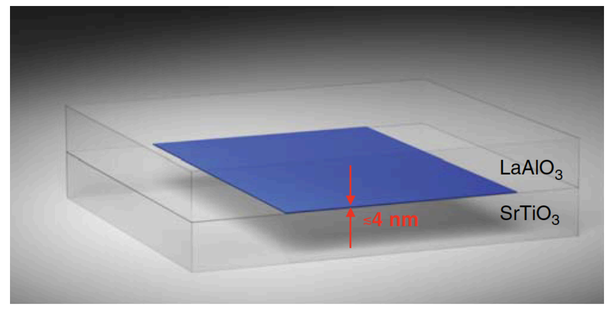

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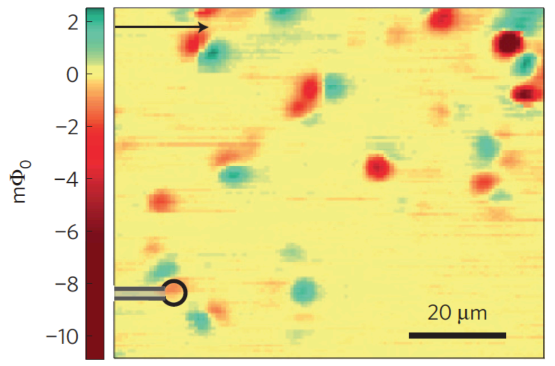

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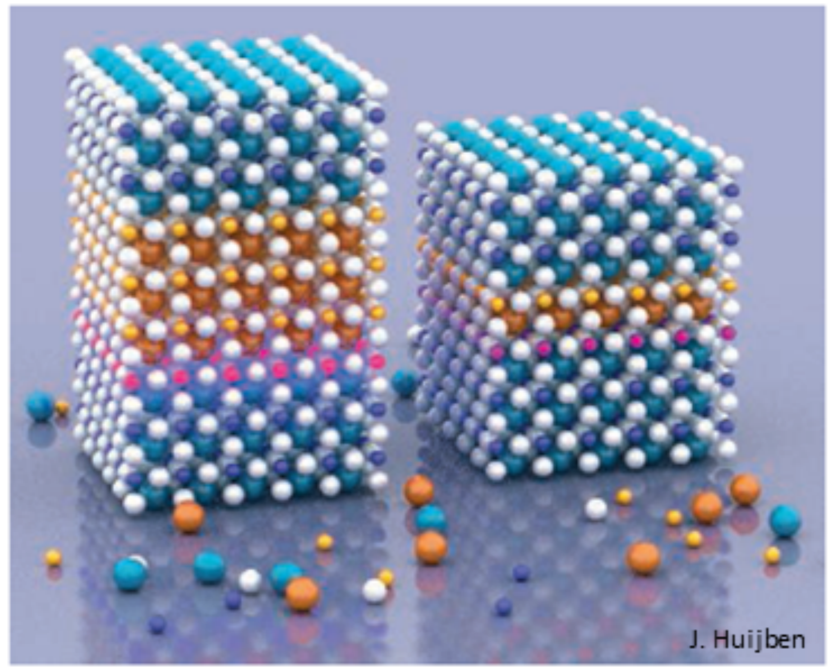
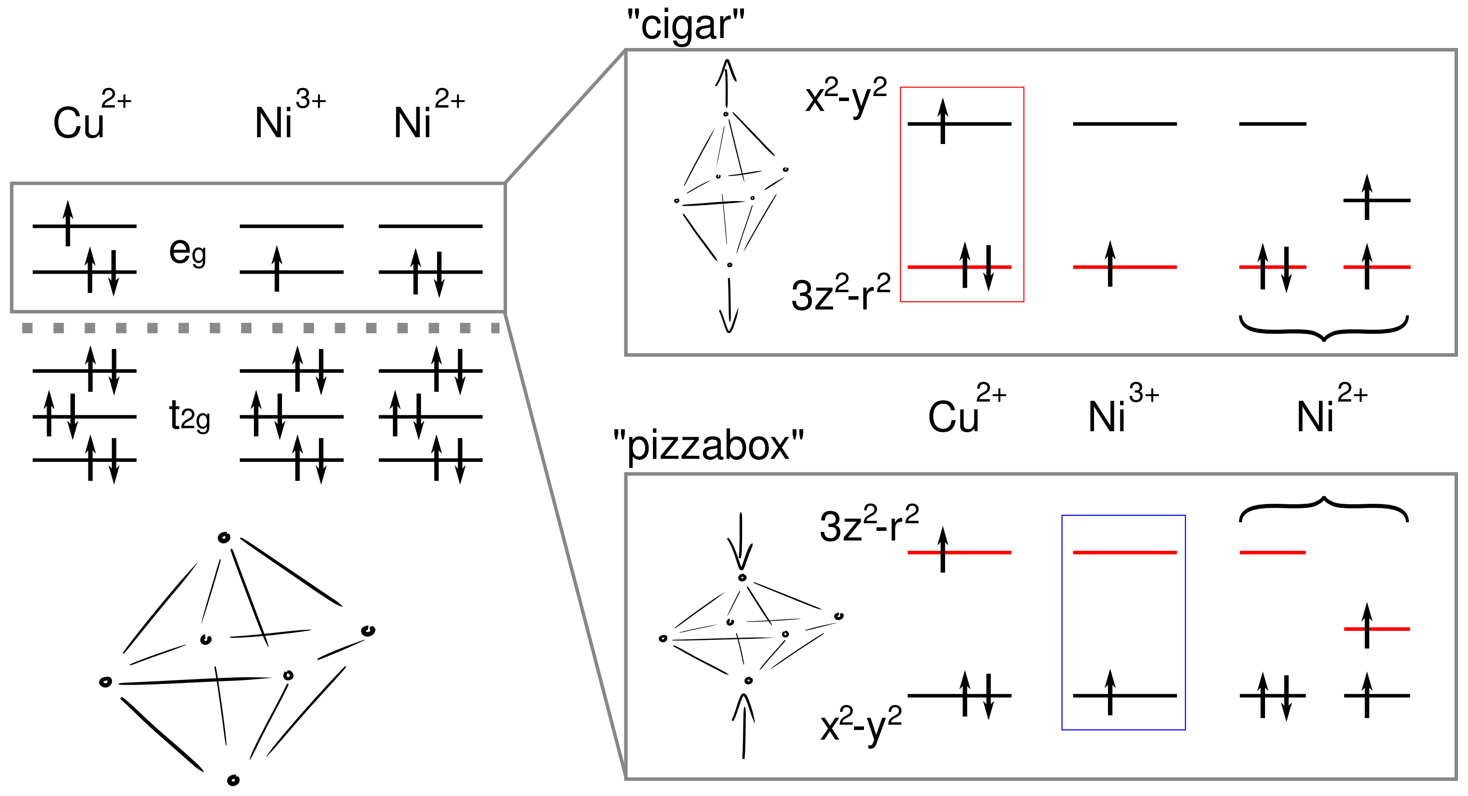


thickness-induced metal-insulator transitions

e$_g$

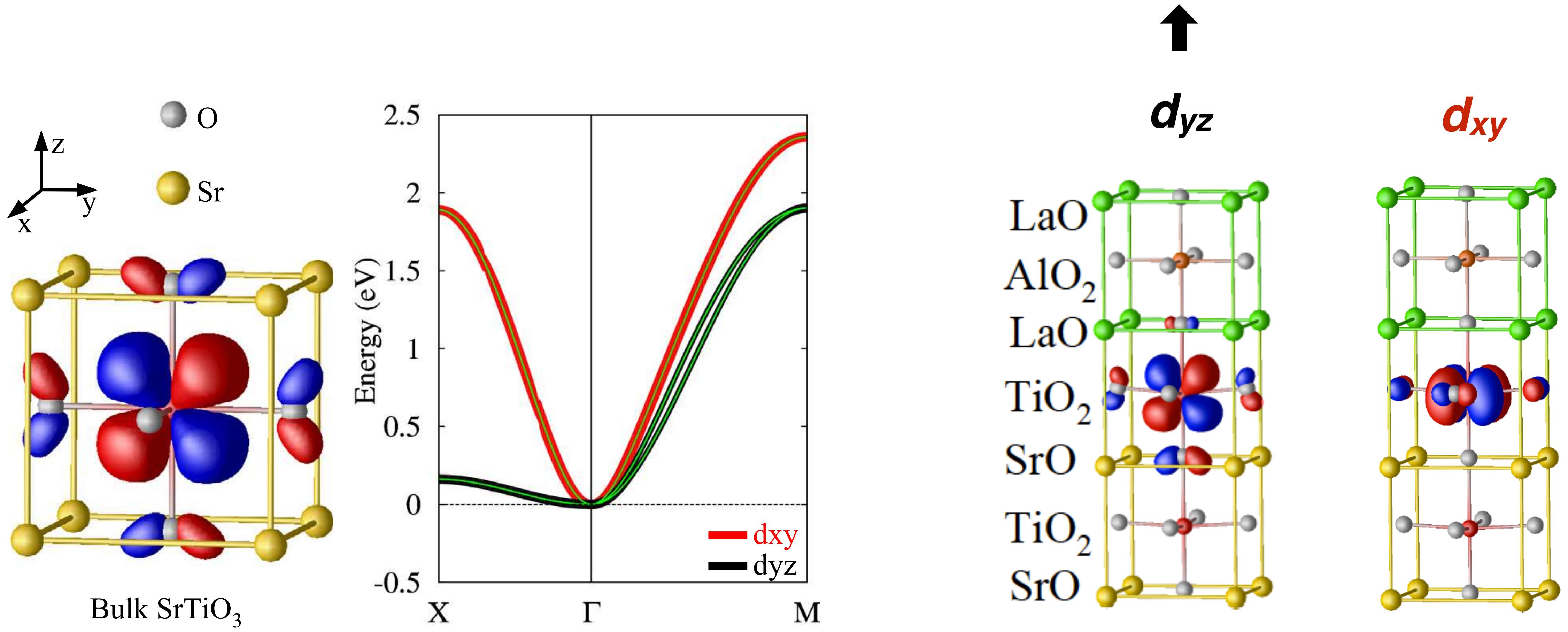


cubic

tetragonal

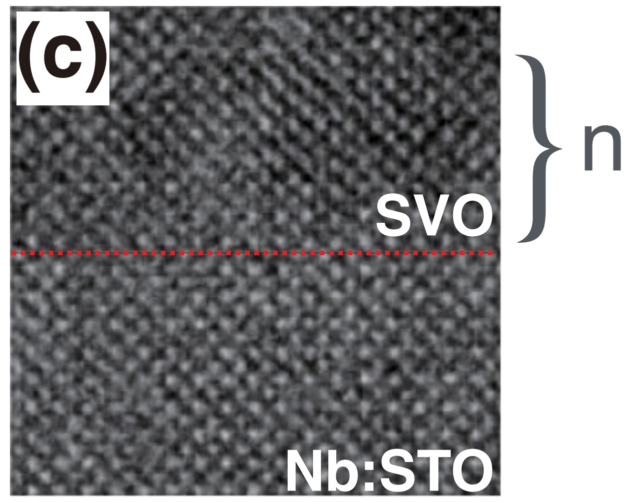
Hansmann, *et al.*, PRL (2009)

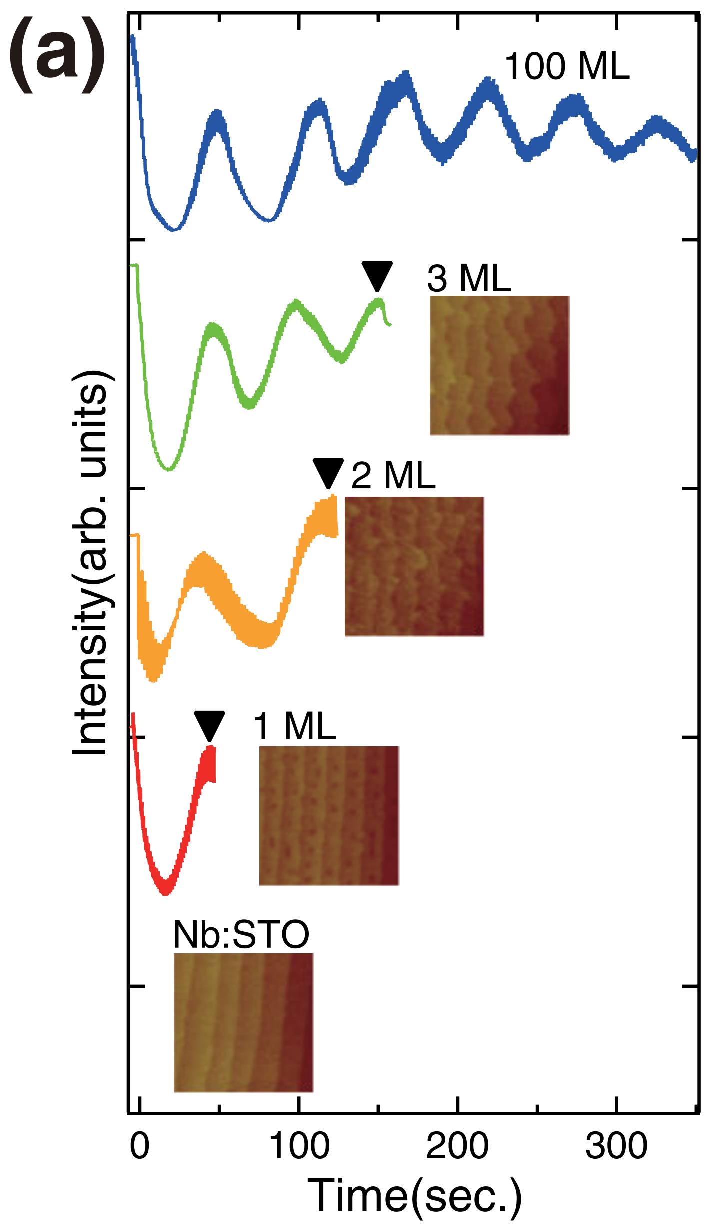
t$_{2g}$



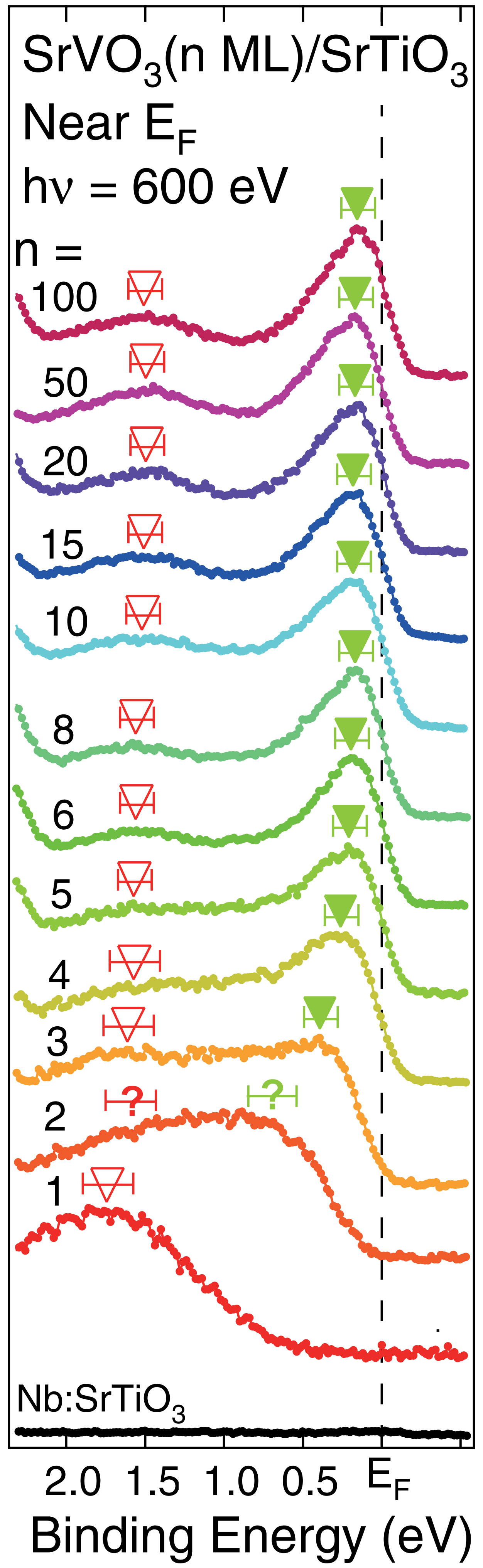
Thickness-induced metal-insulator transition in vanadium think films

- thin films of good-old-friend $SrVO_3$ on $SrTiO_3$
- weight at E_F disappears for small values of n





Yoshimatsu, *et al.*, PRL (2010)



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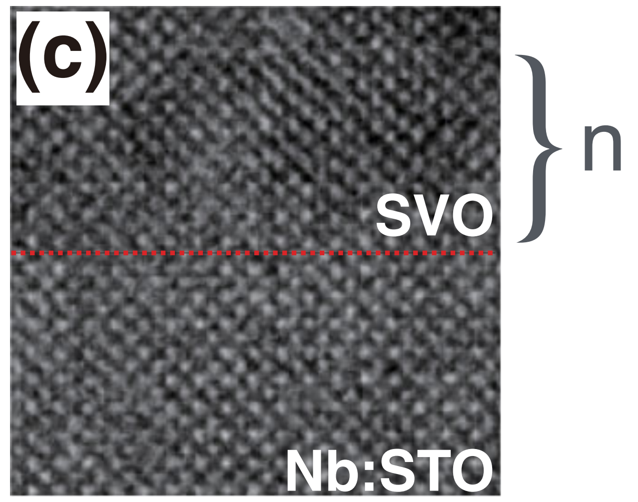
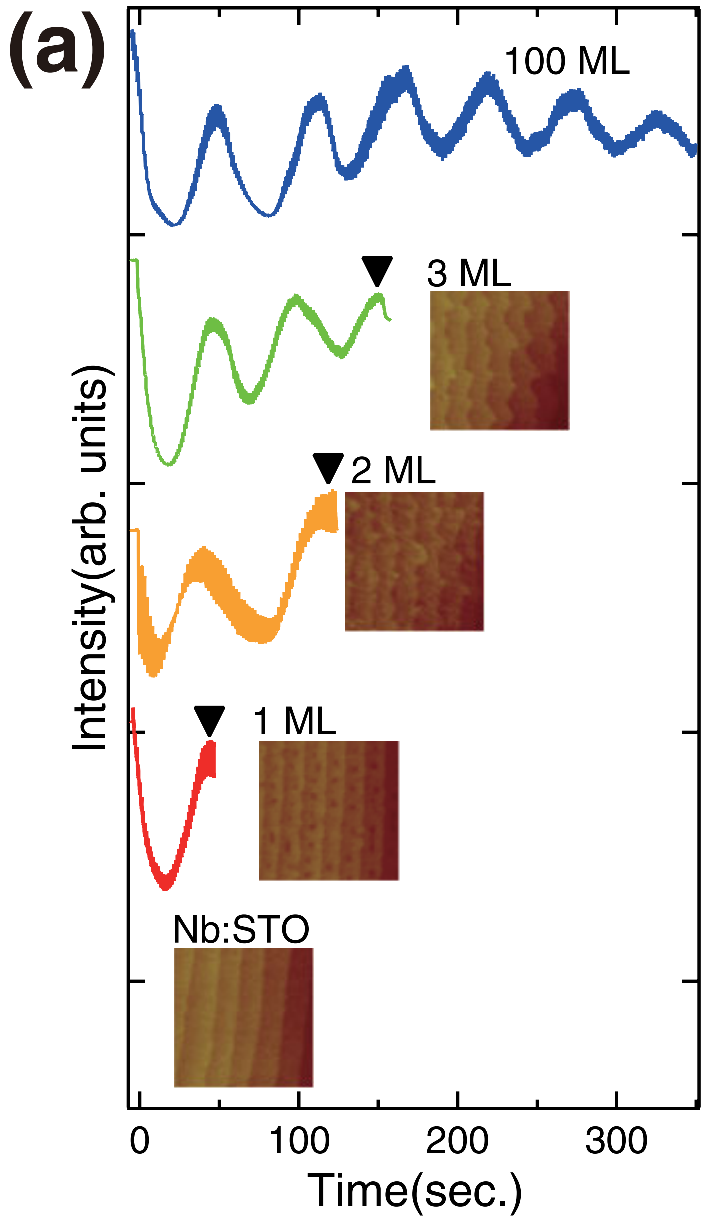
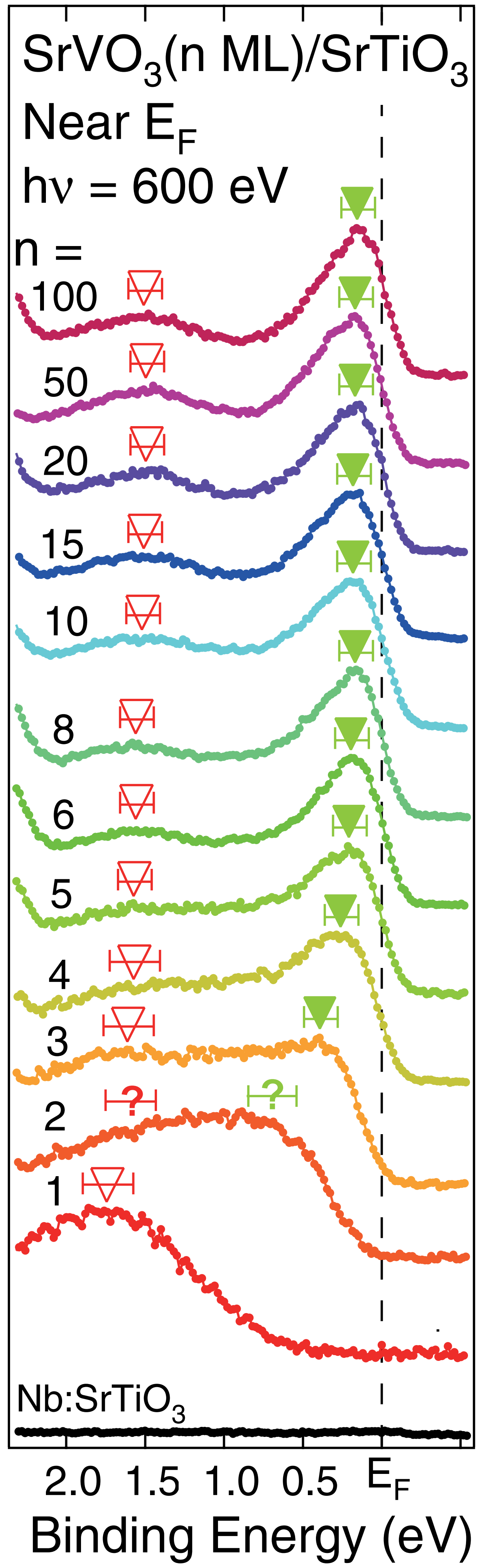
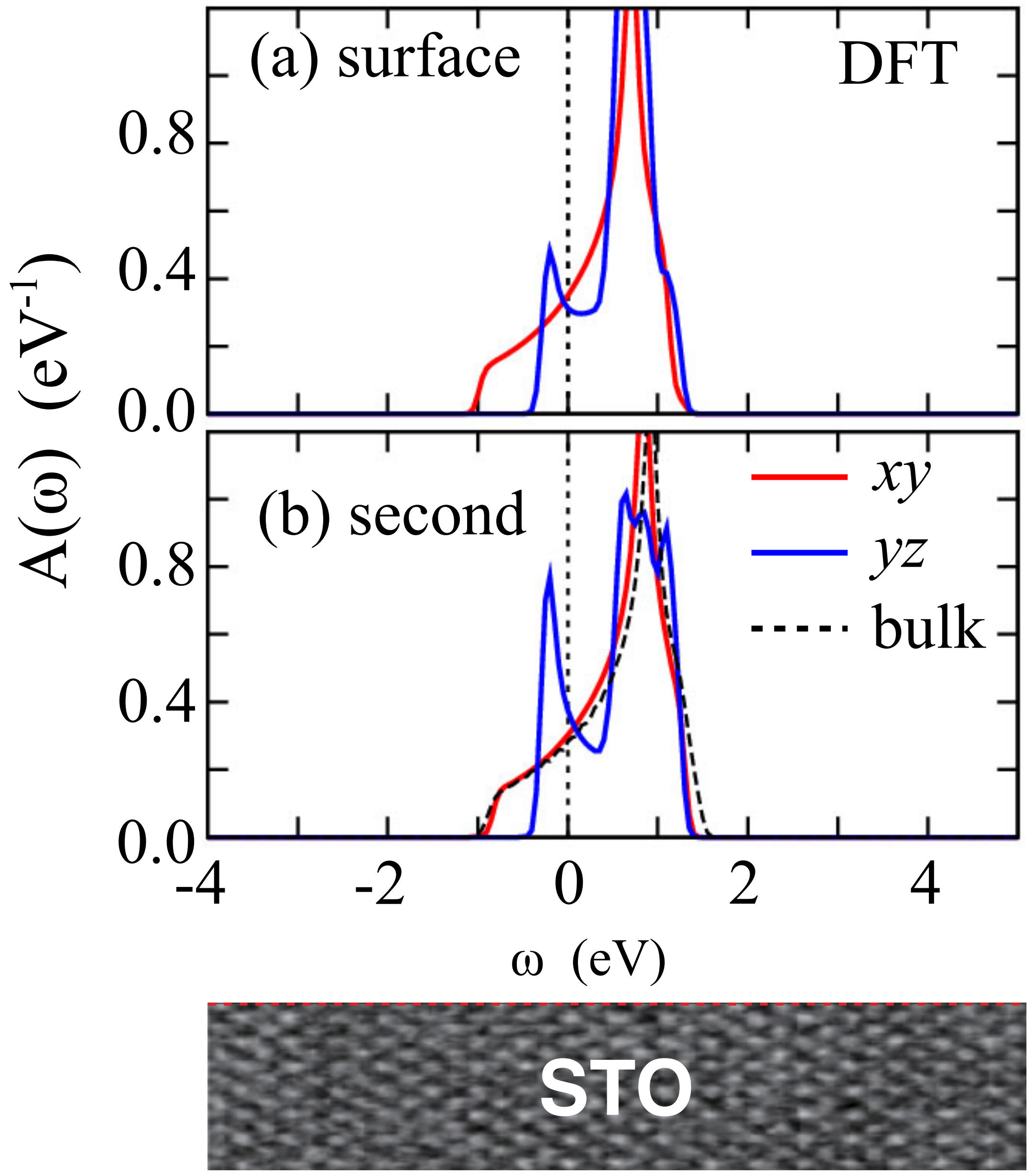
- SVO thin films in DFT (n=2)
- splitting of the t_{2g}









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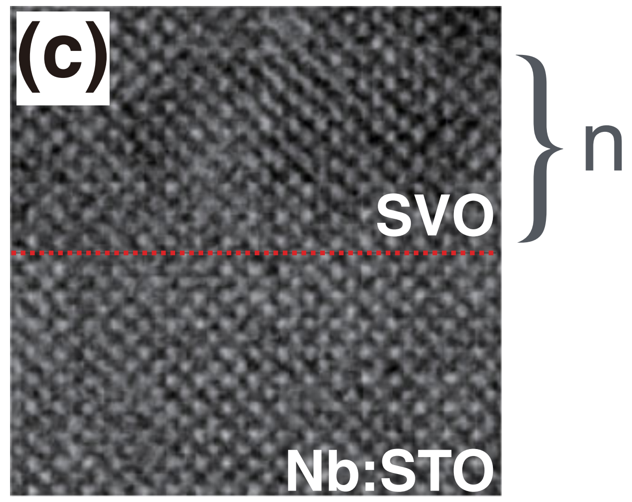

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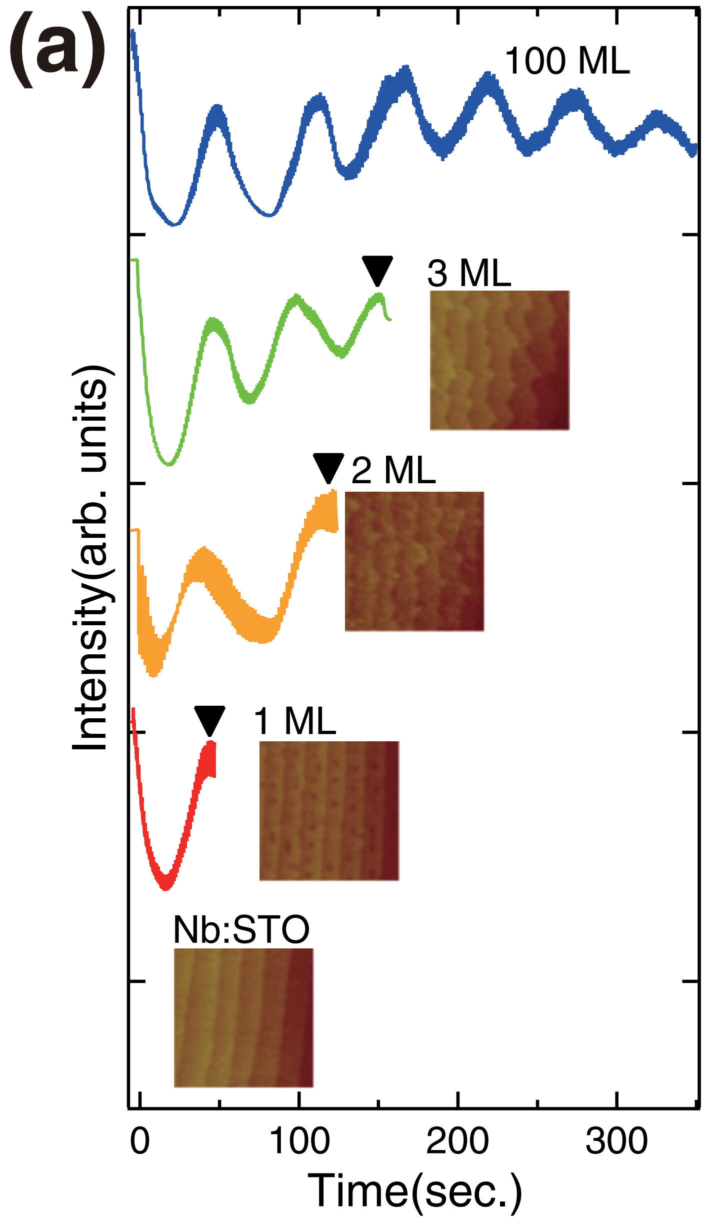

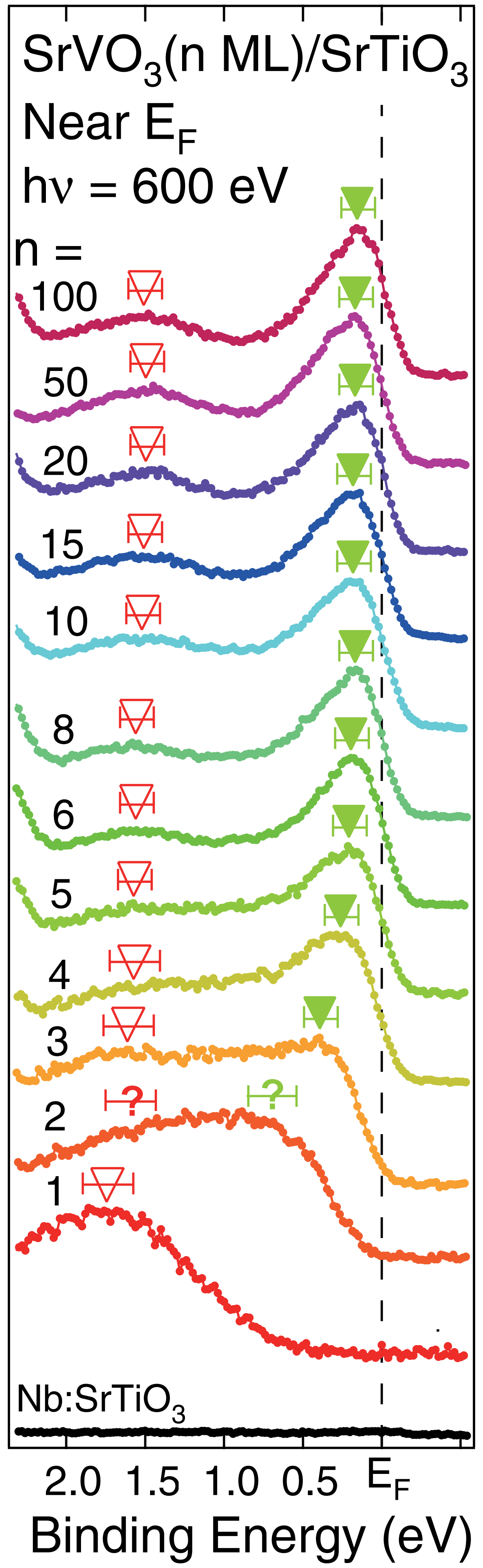

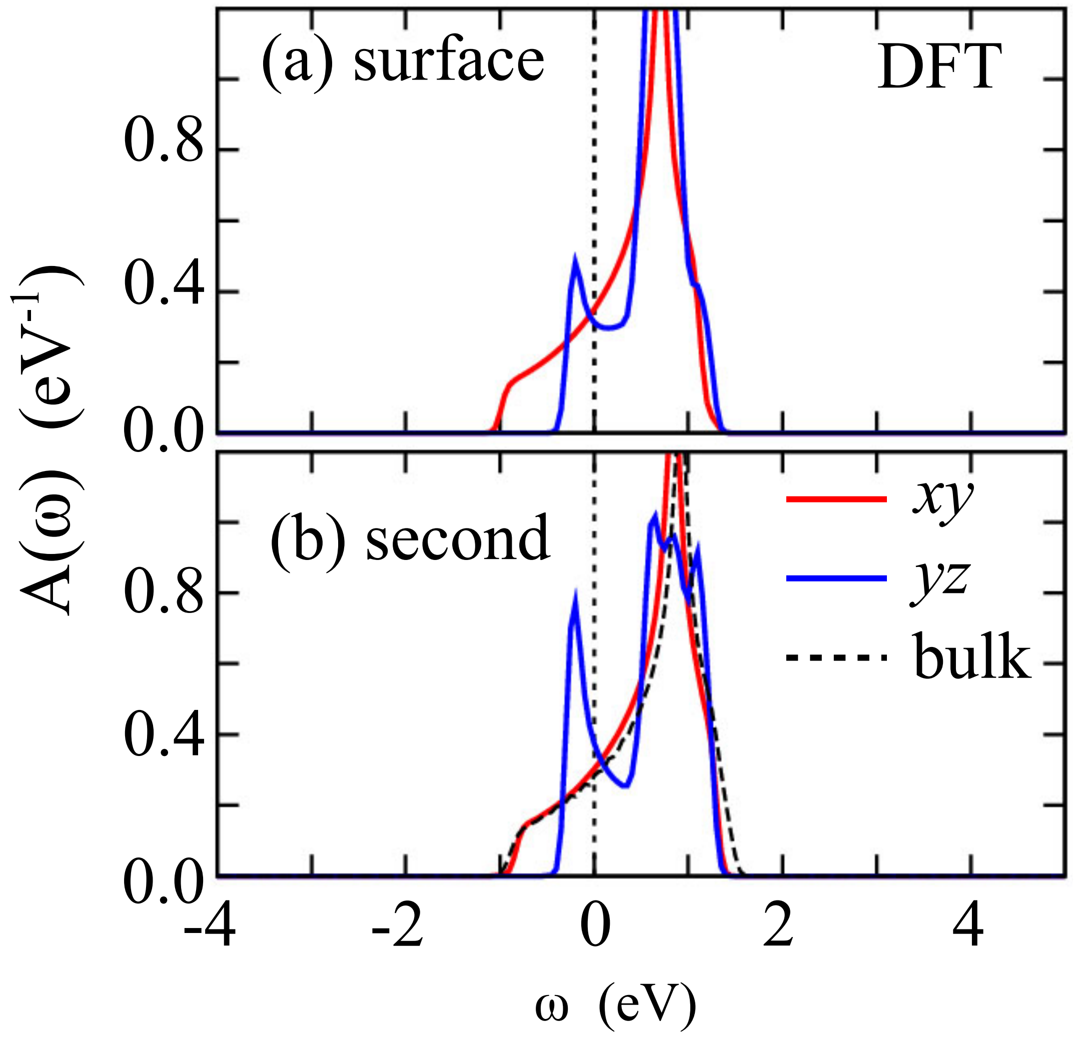

DFT+DMFT?

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Device concept?

- orbital polarization easy to switch ON and OFF!
  (thickness, pressure, strain, temperature, gating,…)
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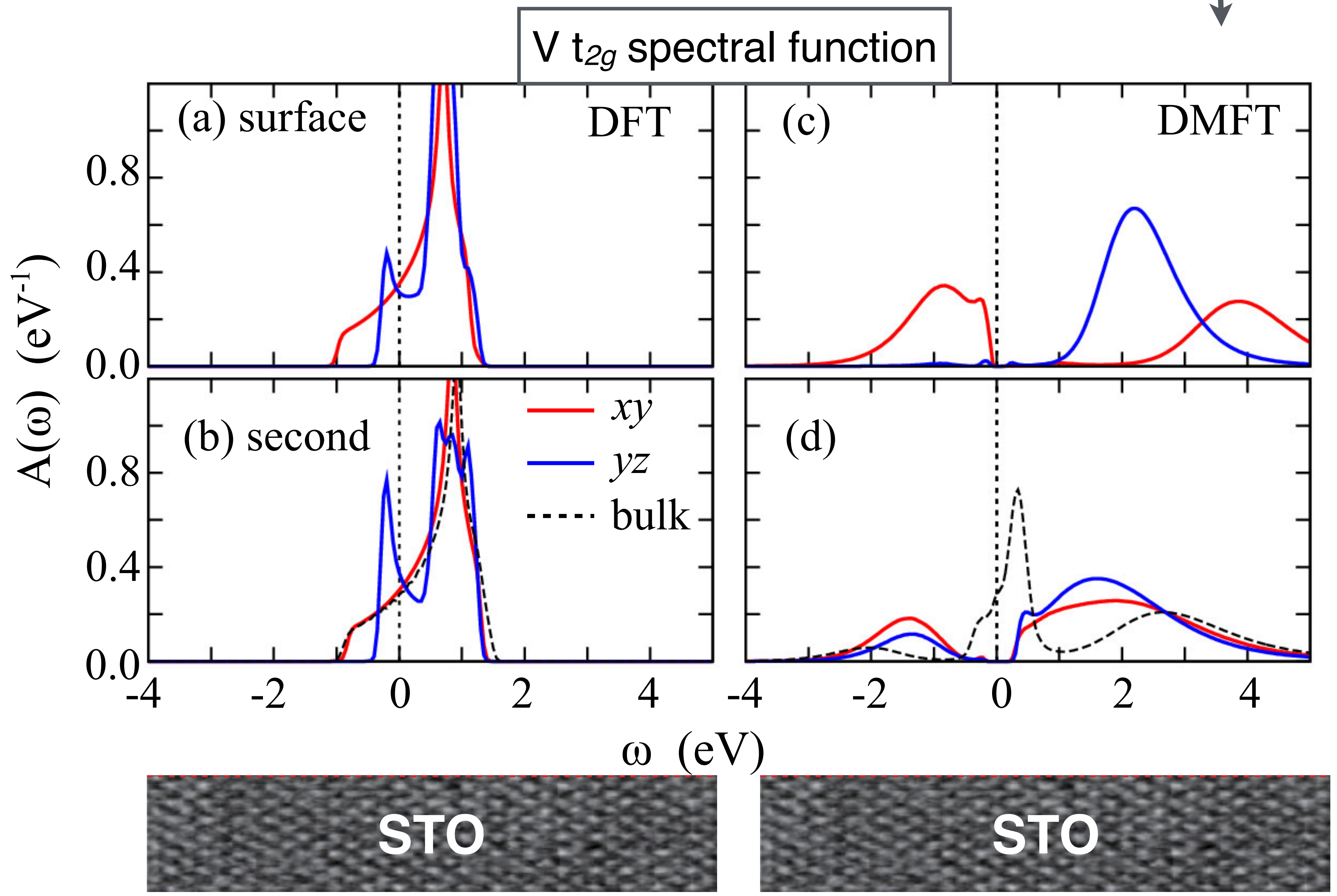
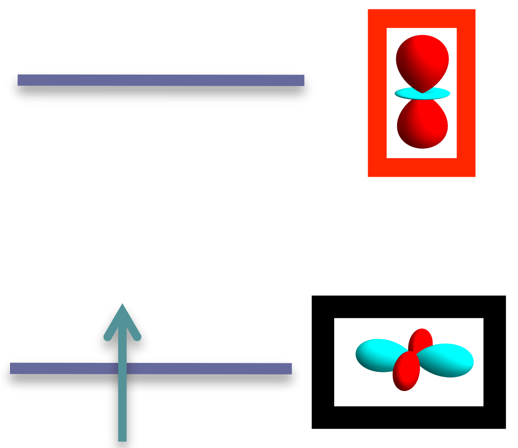


PRL 114, 246401 (2015) PHYSICAL REVIEW LETTERS week ending 19 JUNE 2015

Electronics with Correlated Oxides: $SrVO_3/SrTiO_3$ as a Mott Transistor

Zhicheng Zhong,[1] Markus Wallerberger,[1] Jan M. Tomczak,[1] Ciro Taranto,[1] Nicolaus Parragh,[2] Alessandro Toschi,[1] Giorgio Sangiovanni,[2] and Karsten Held[1]

$$\Delta_{\text{eff}}^{t_{2g}} = \Delta_{\text{DFT}}^{t_{2g}} + \text{Re}\Sigma_{yz/xz}(\omega \to 0) - \text{Re}\Sigma_{xy}(\omega \to 0)$$



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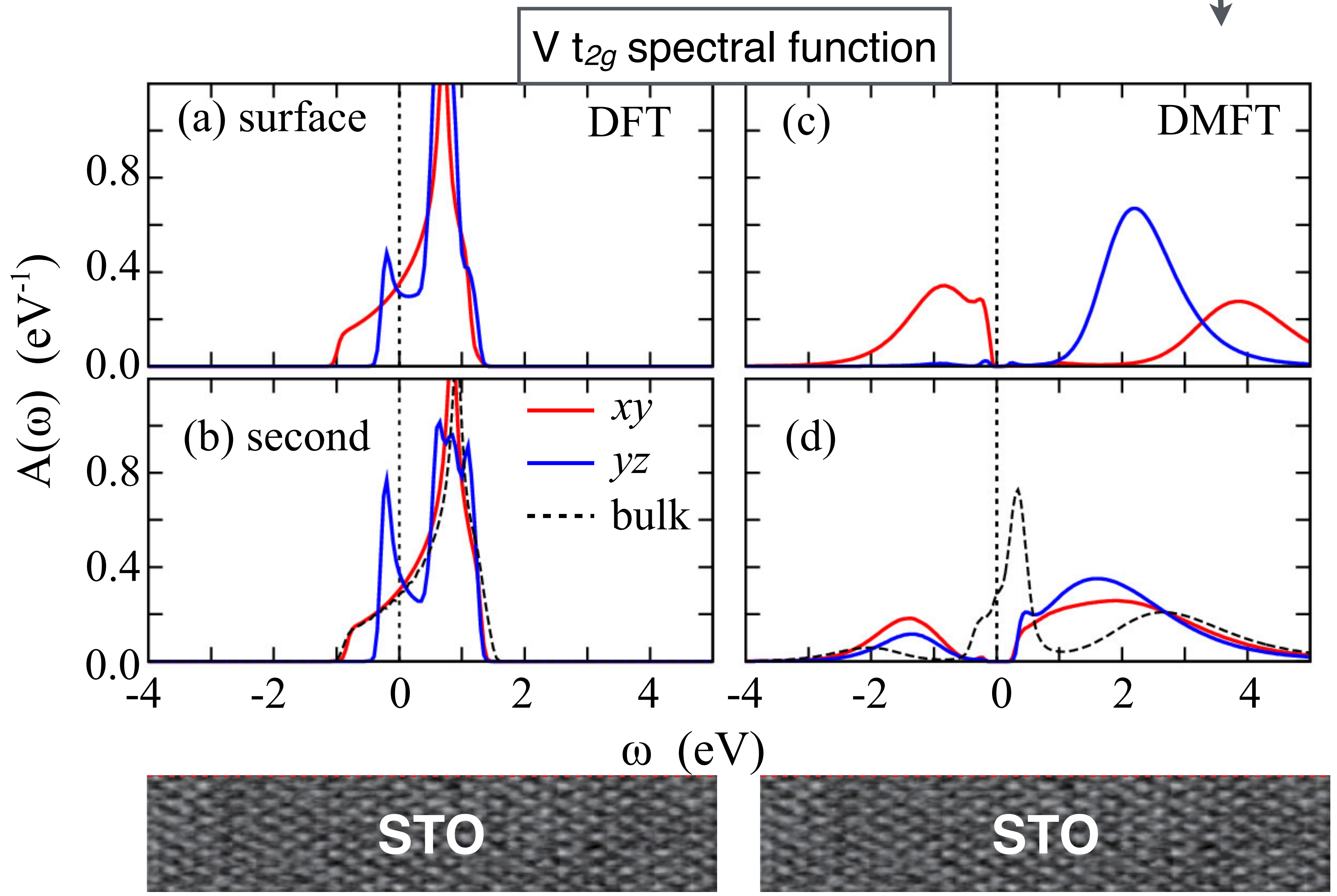

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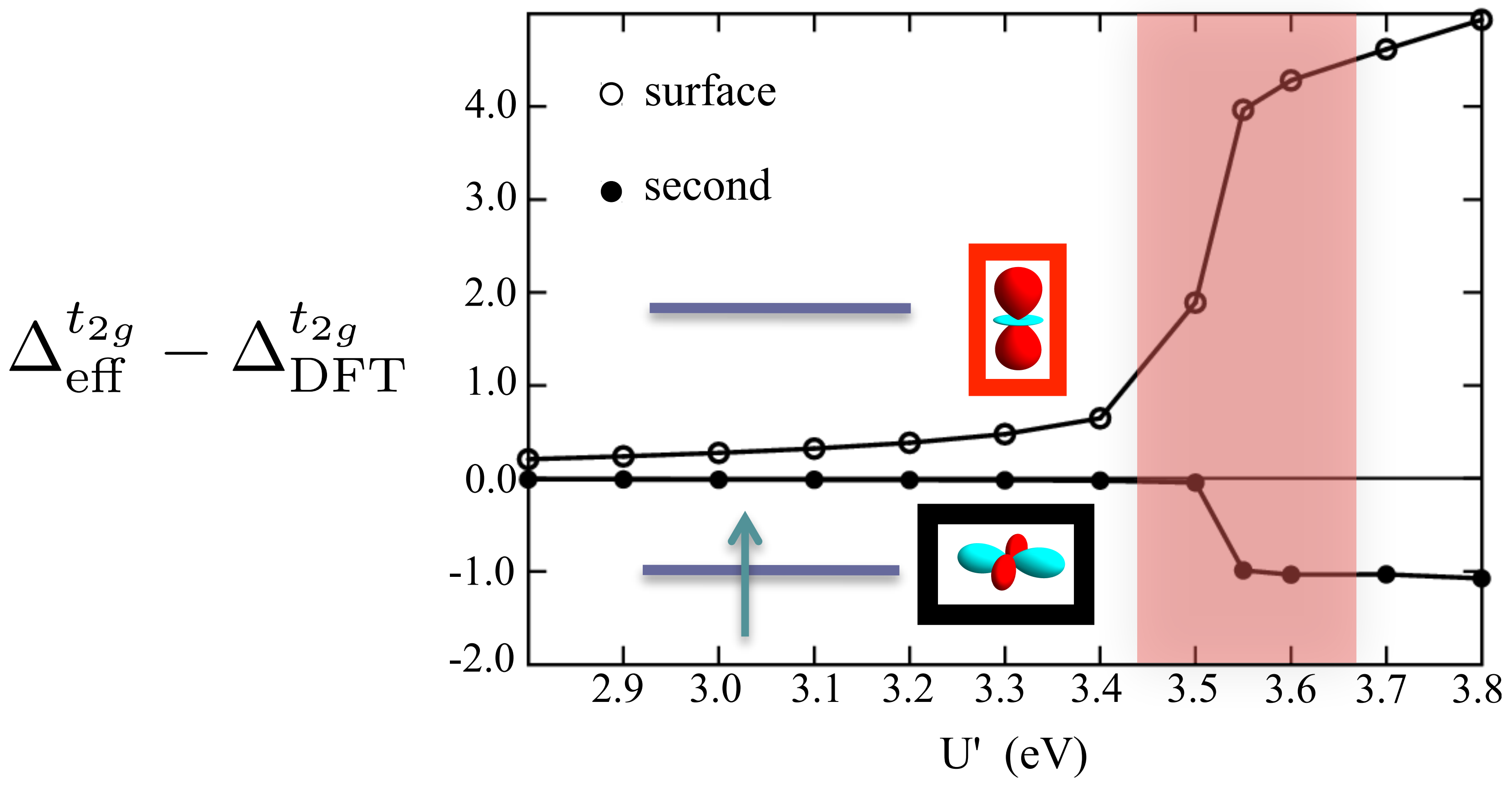

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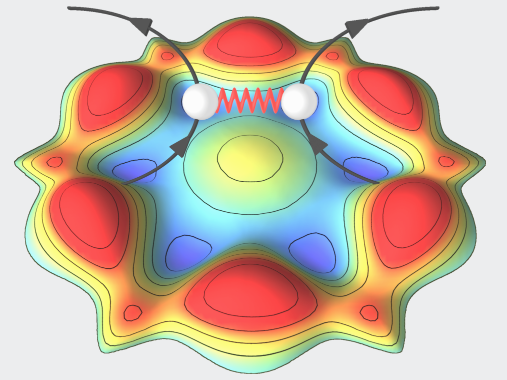

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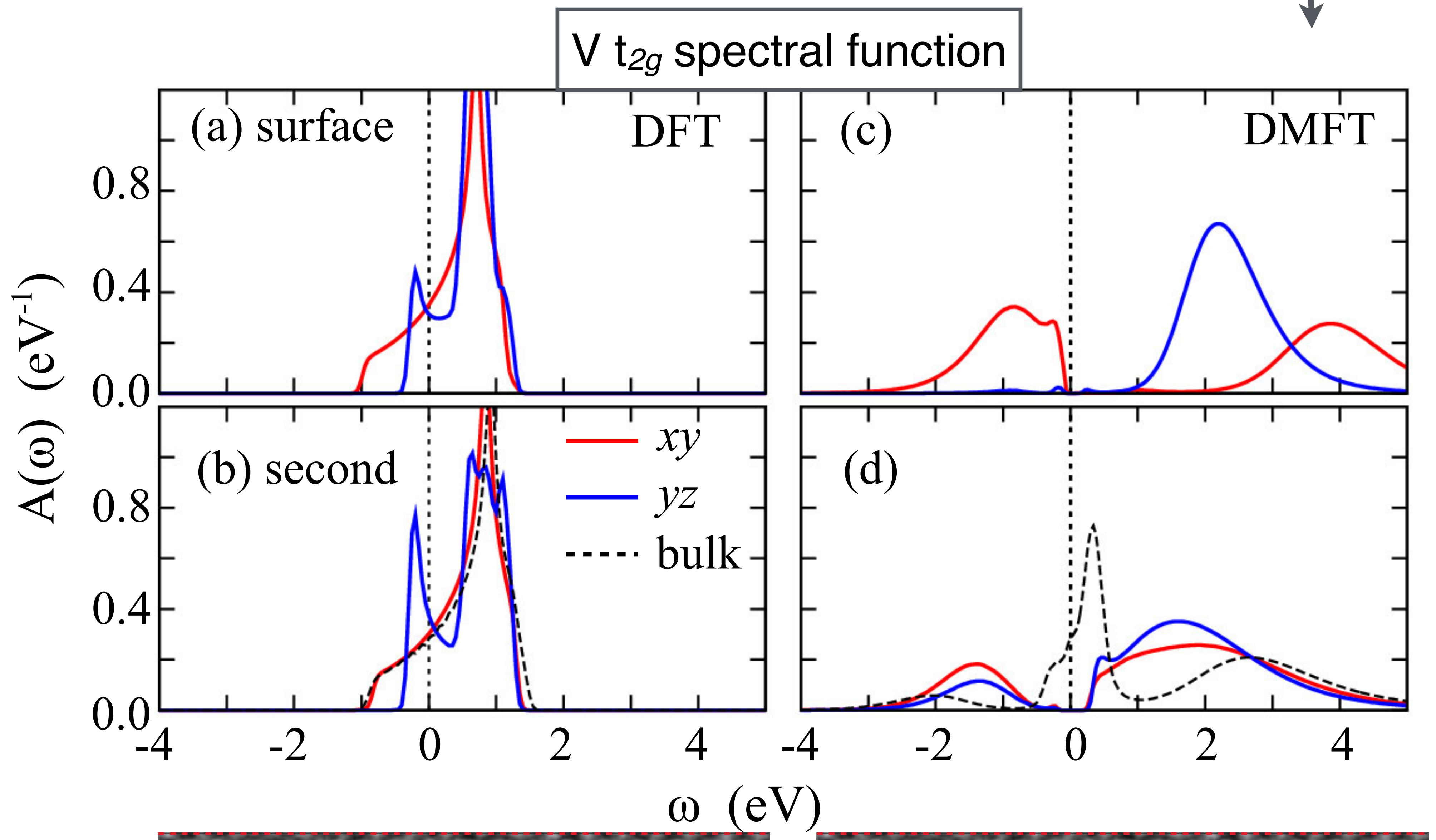

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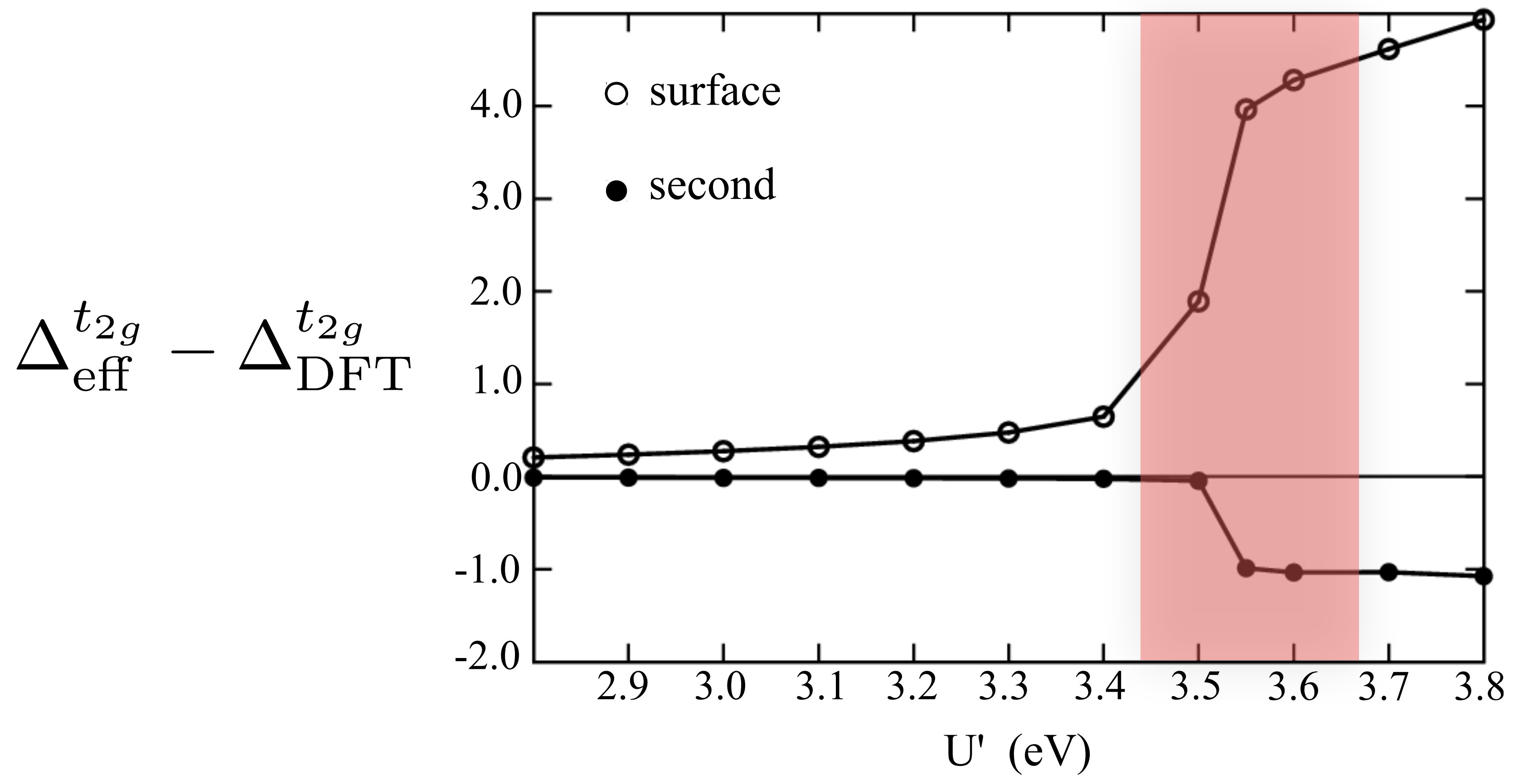
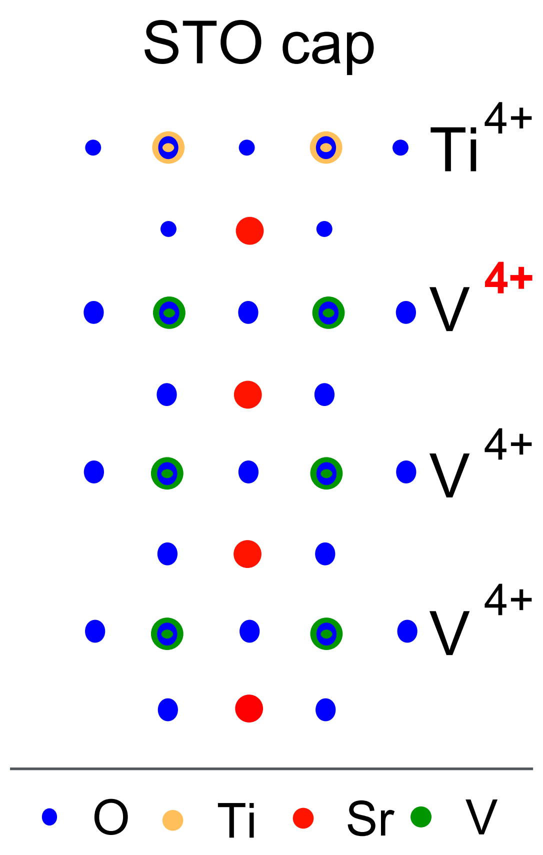


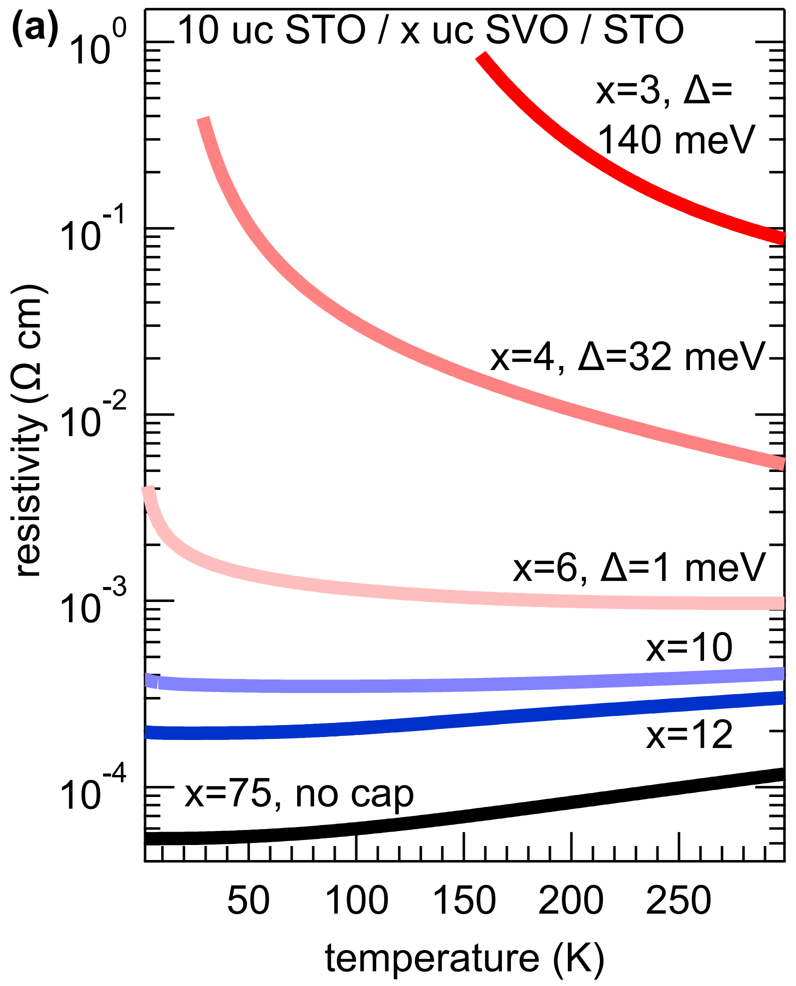
Julius-Maximilians-
UNIVERSITÄT
WÜRZBURG

Surface of SVO thin films

- termination for $SrVO_3$ fims on $SrTiO_3$
- VO_2 + $\sqrt{2} \times \sqrt{2}$ oxygen reconstruction
- solution: capping!



P. Scheiderer, PhD Thesis (Würzburg)



- surprising result:

  critical thickness much bigger than

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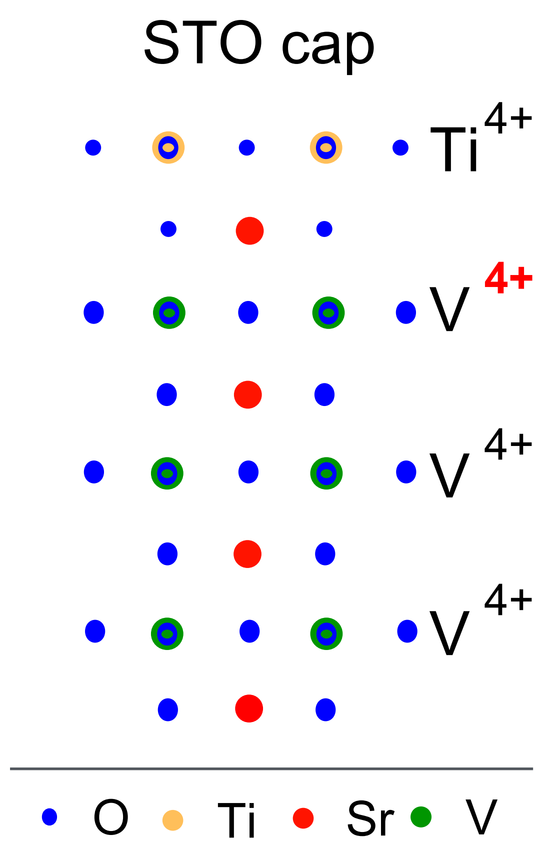

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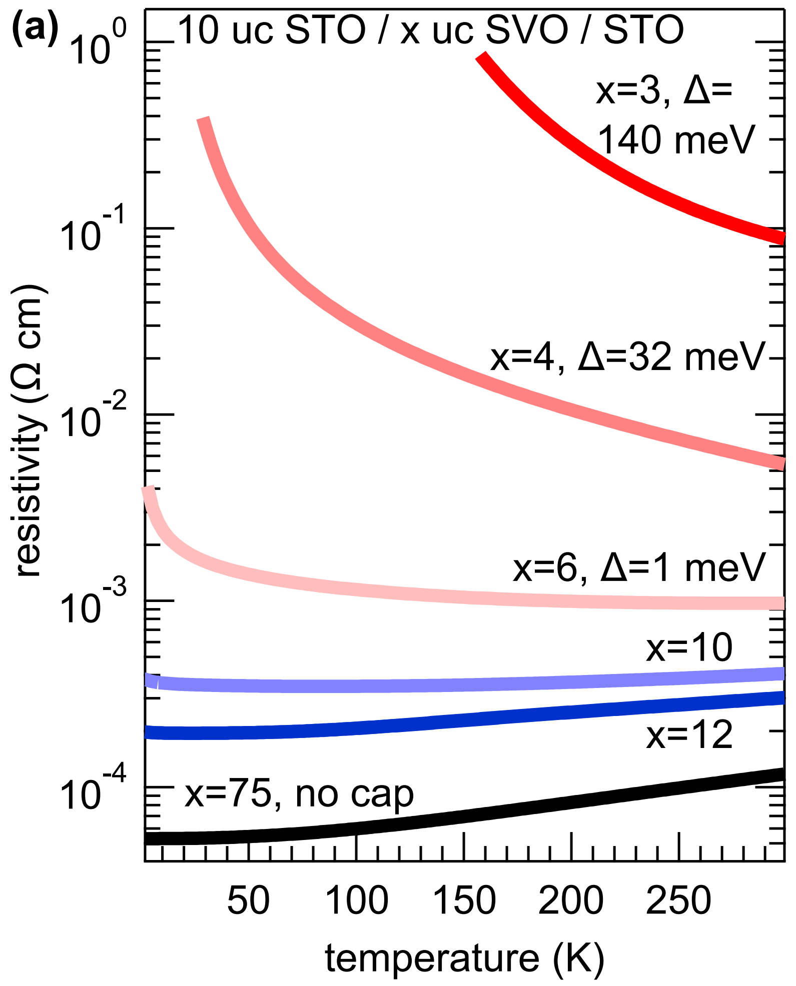

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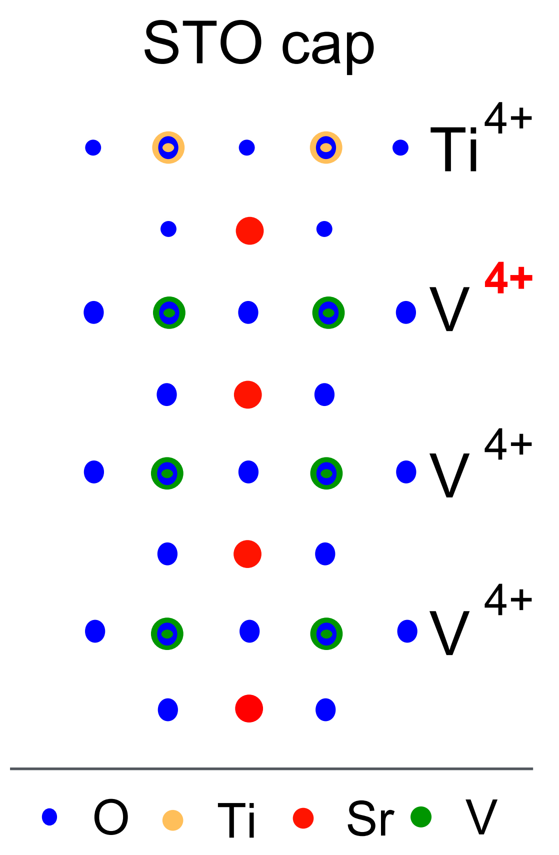

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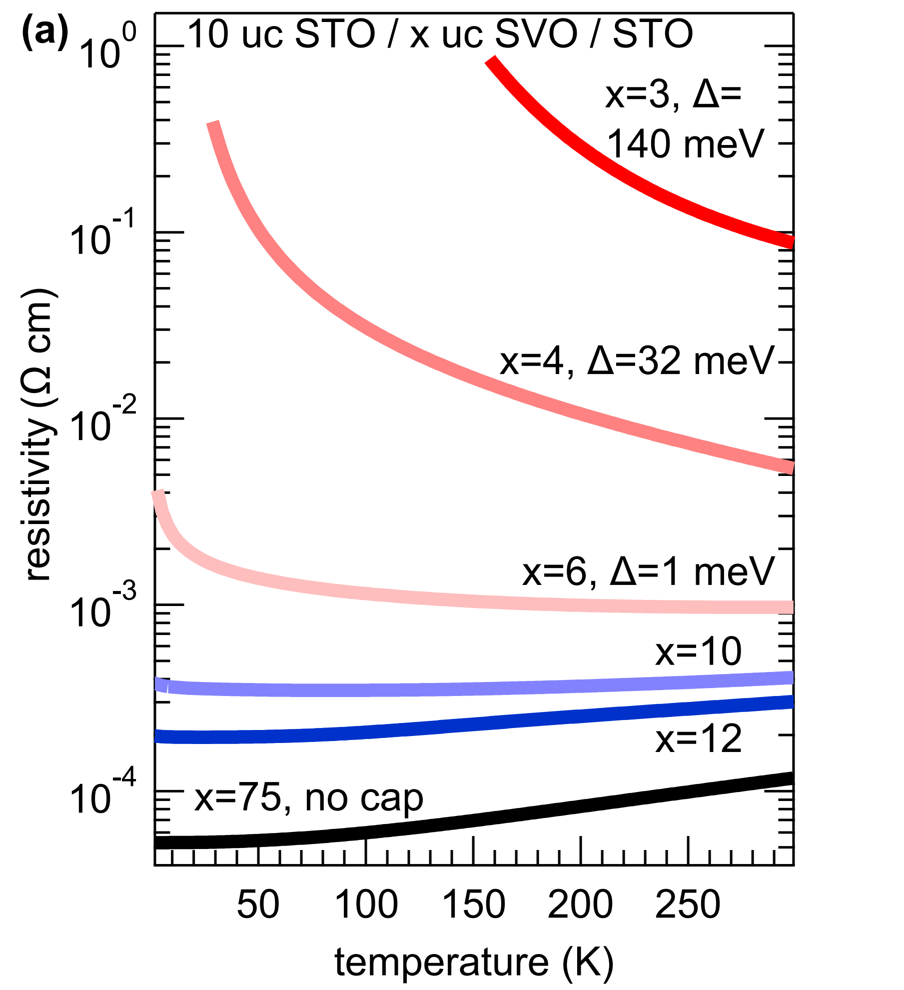

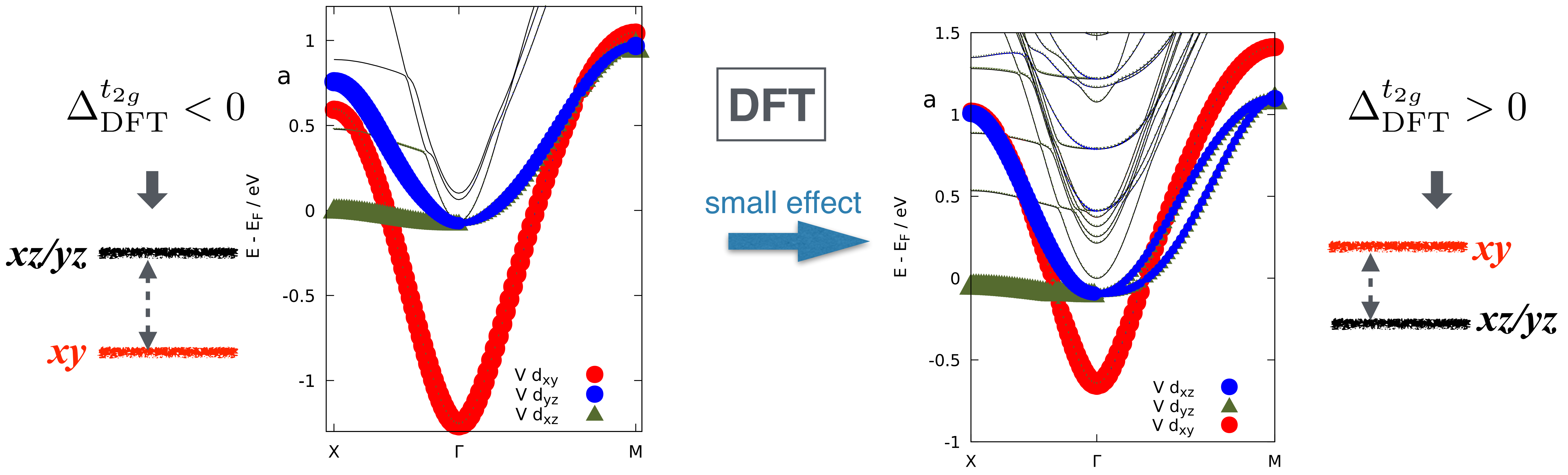

SrO termination (i.e. complete octahedra)

ideal VO_2 termination

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DFT by Marius Fuchs (Würzburg)
DFT+DMFT spectra by Matthias Pickem (group of K. Held and J. Tomczak, TU Wien)

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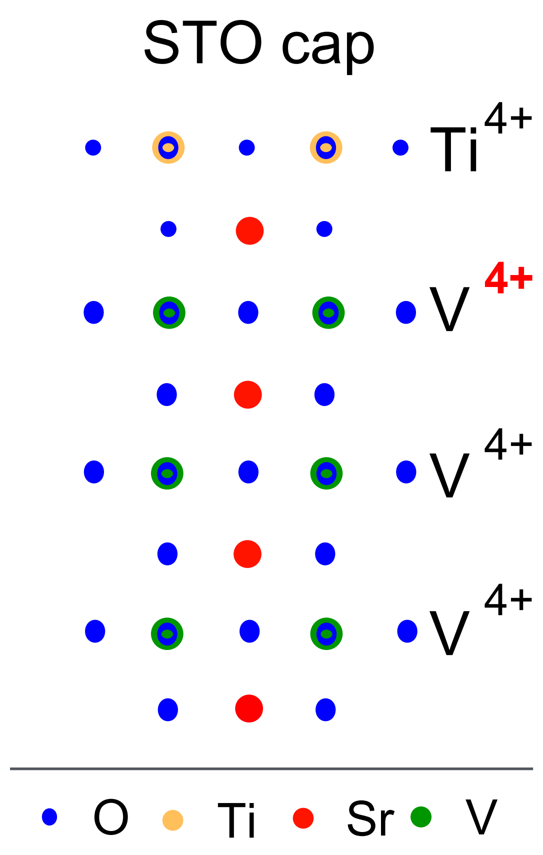

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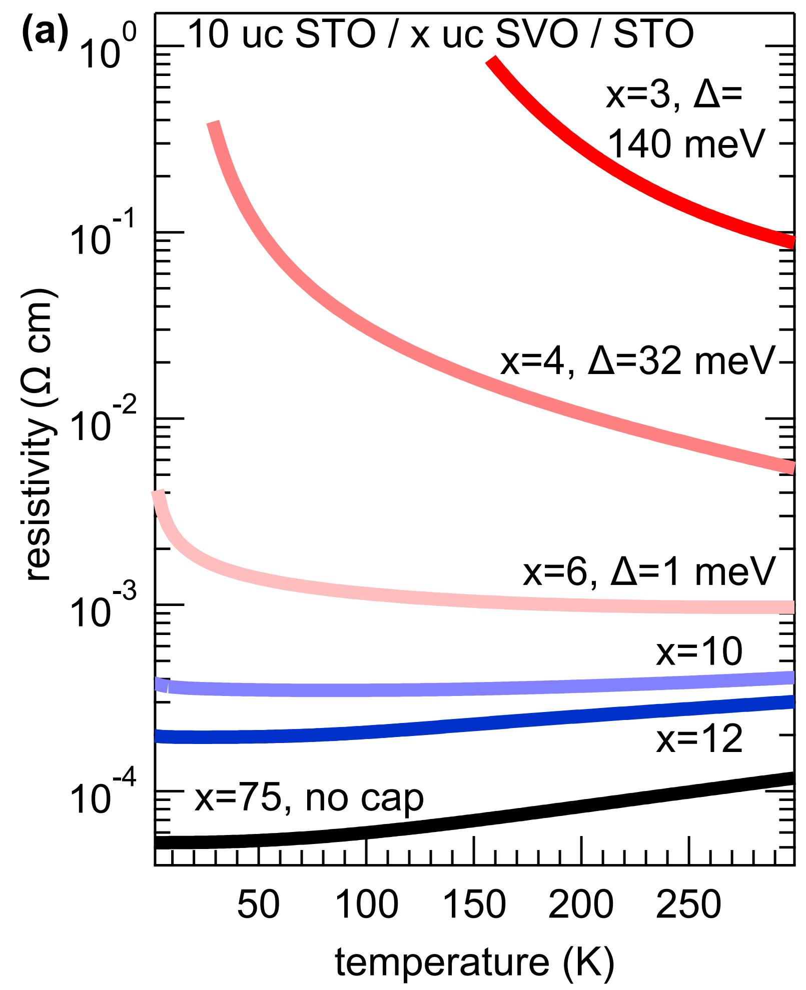

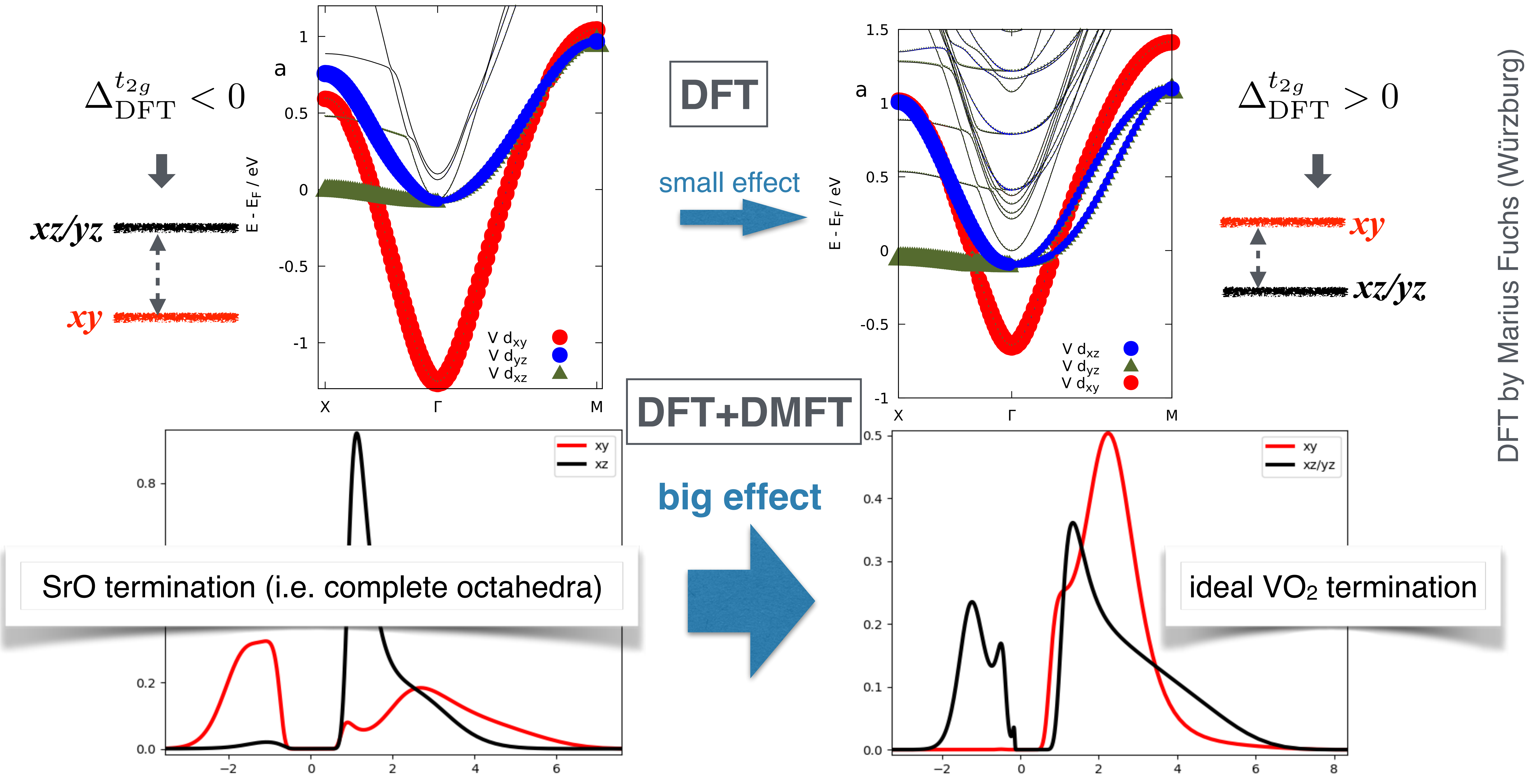

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other examples of thickness induced MIT

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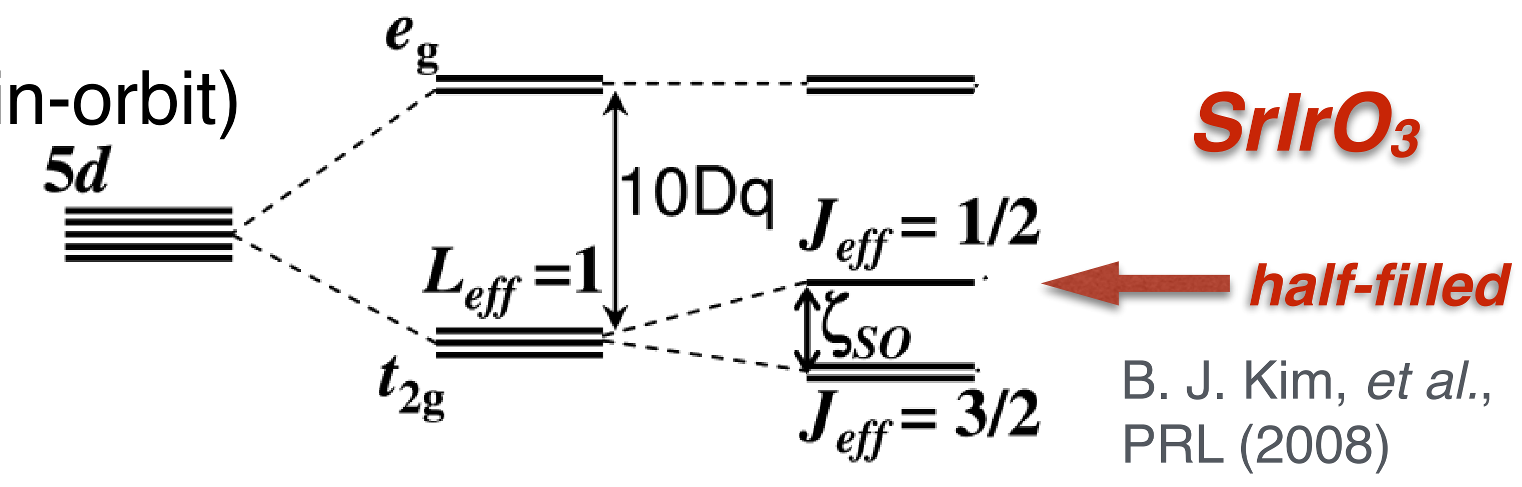

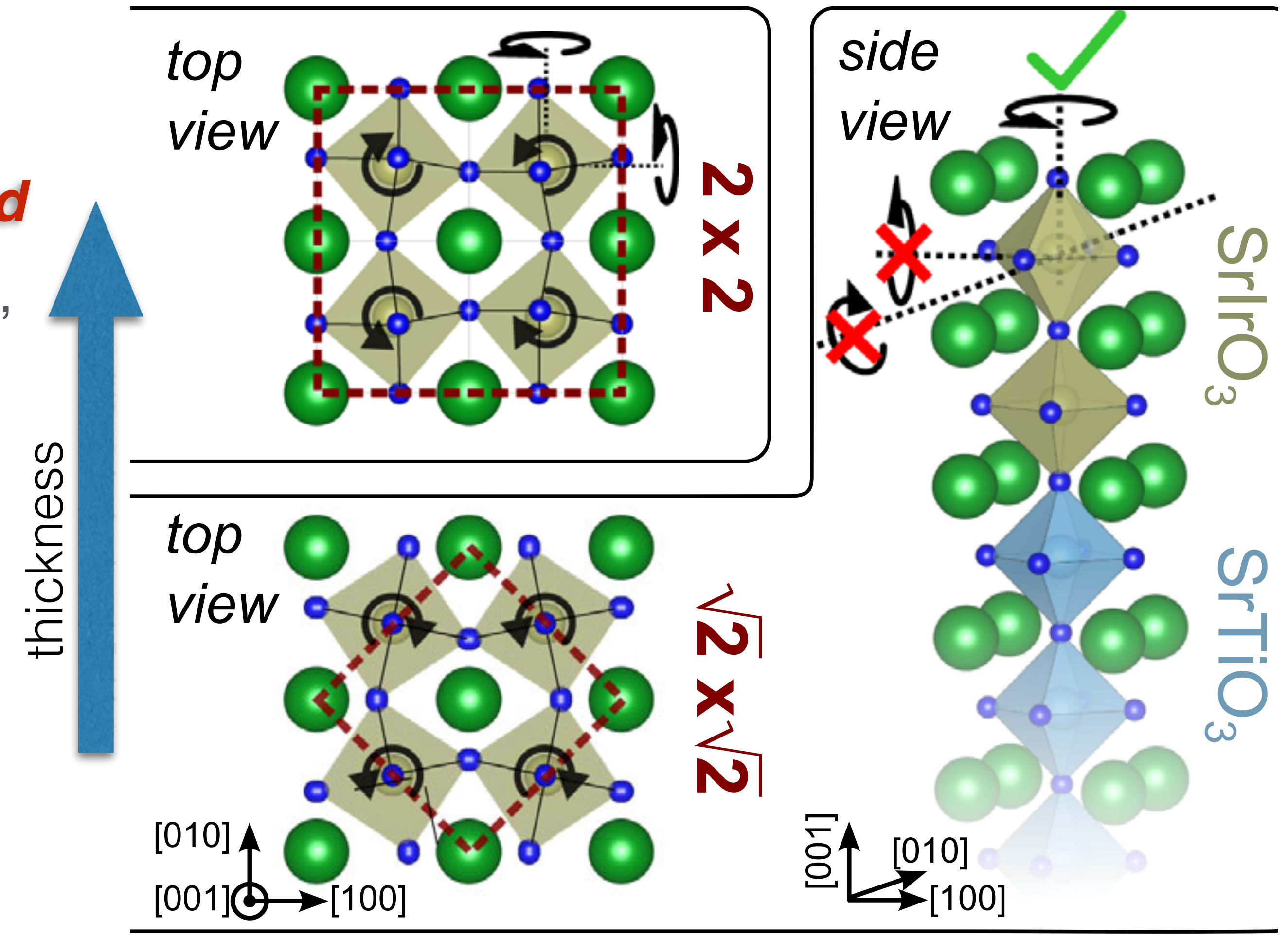

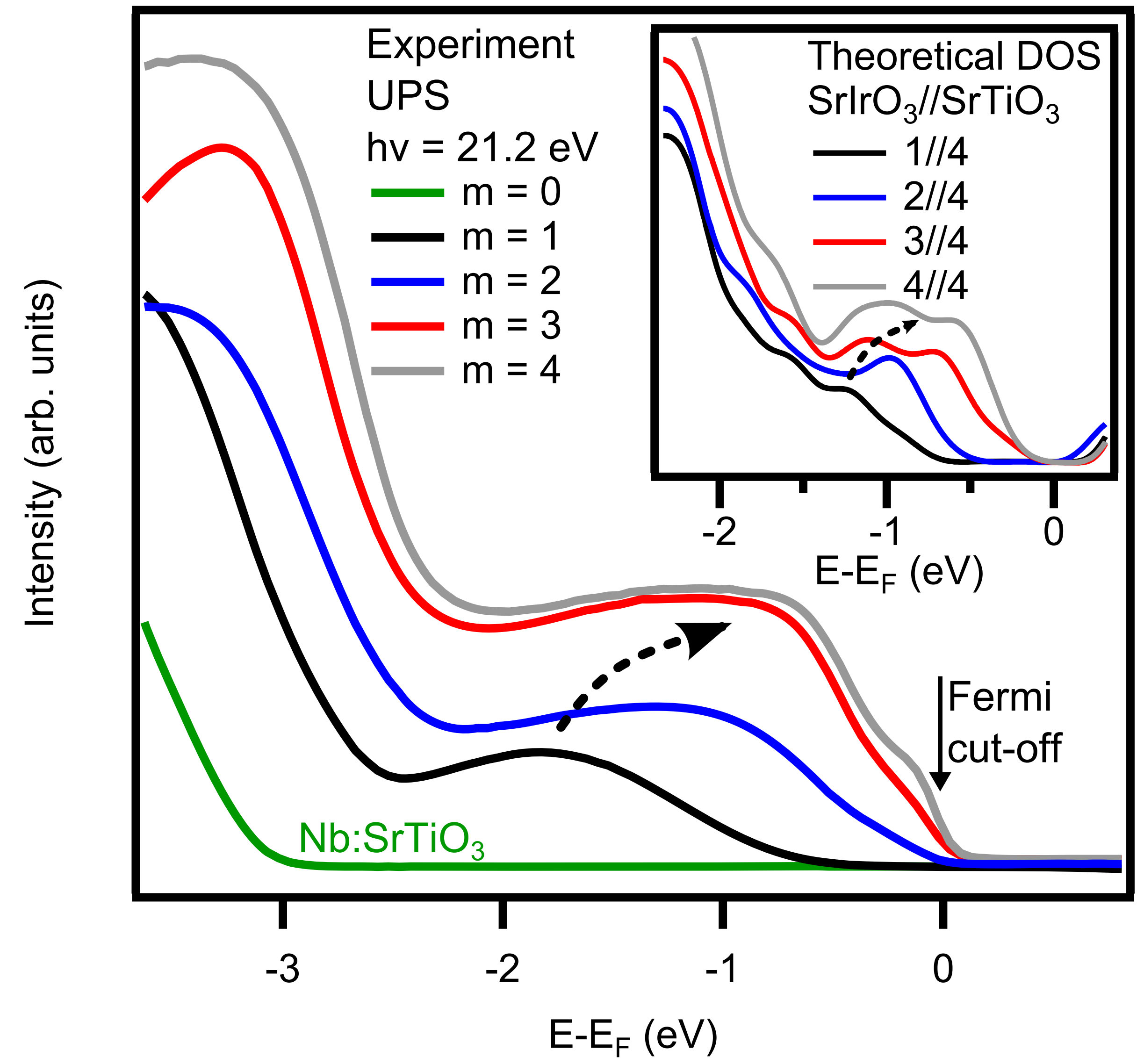

PRL 119, 256404 (2017) PHYSICAL REVIEW LETTERS week ending 22 DECEMBER 2017

Dimensionality-Driven Metal-Insulator Transition in Spin-Orbit-Coupled SrIrO$_3$

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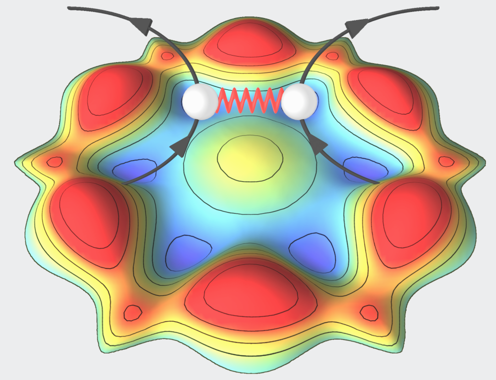

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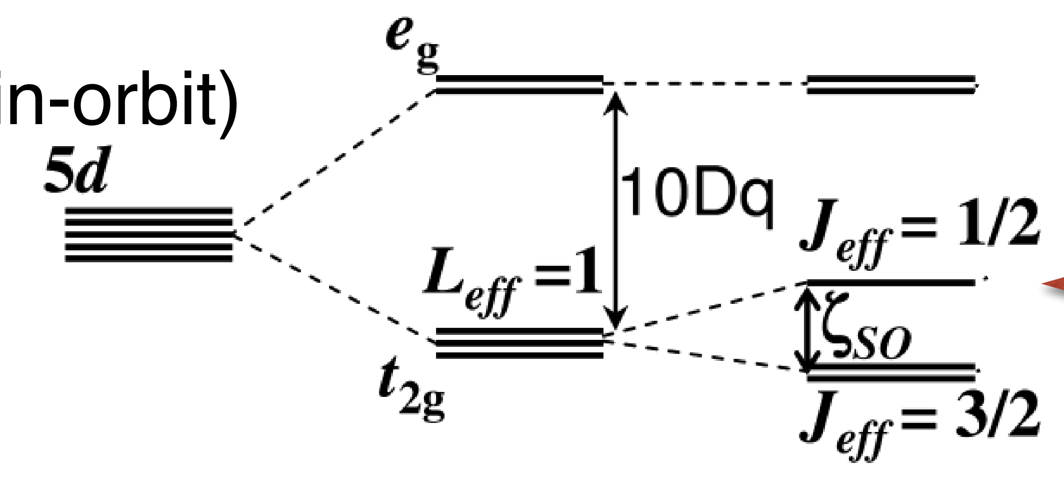

B. J. Kim, *et al.*, PRL (2008)

- mimicking the Ruddlesden-Popper series:

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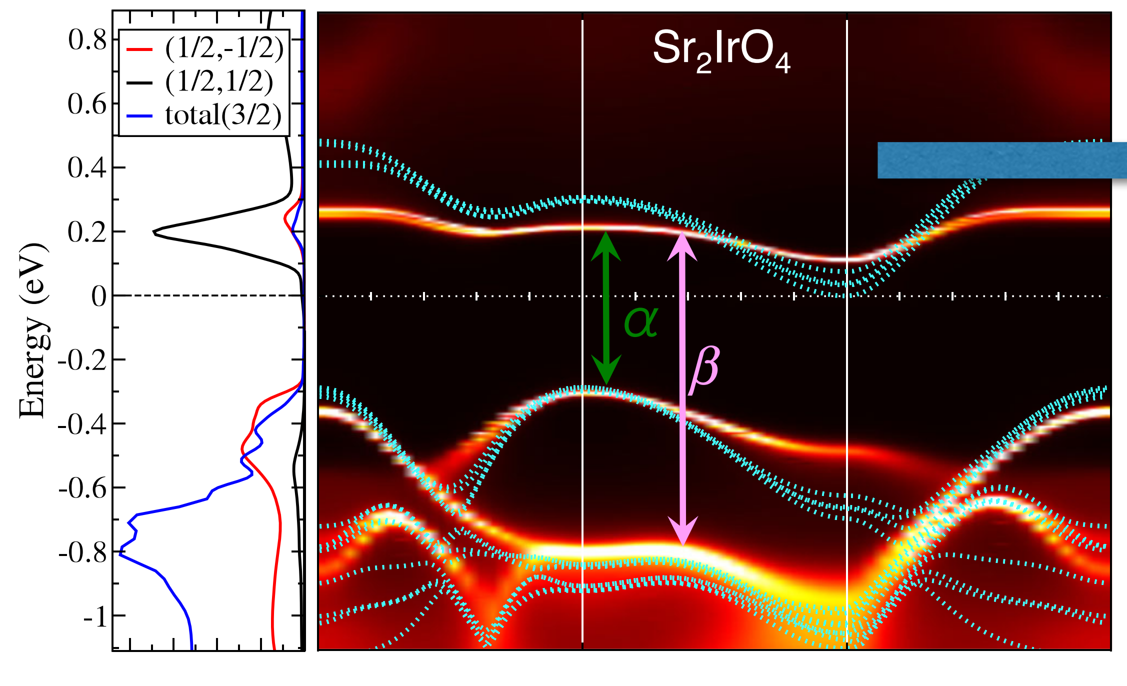

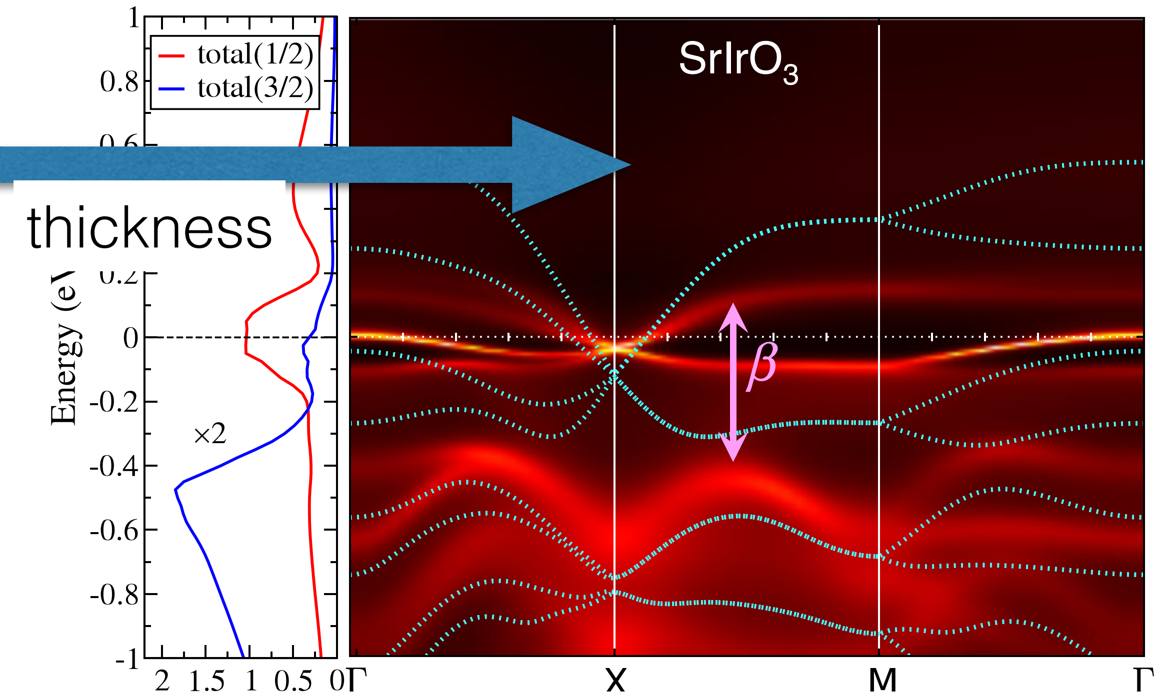

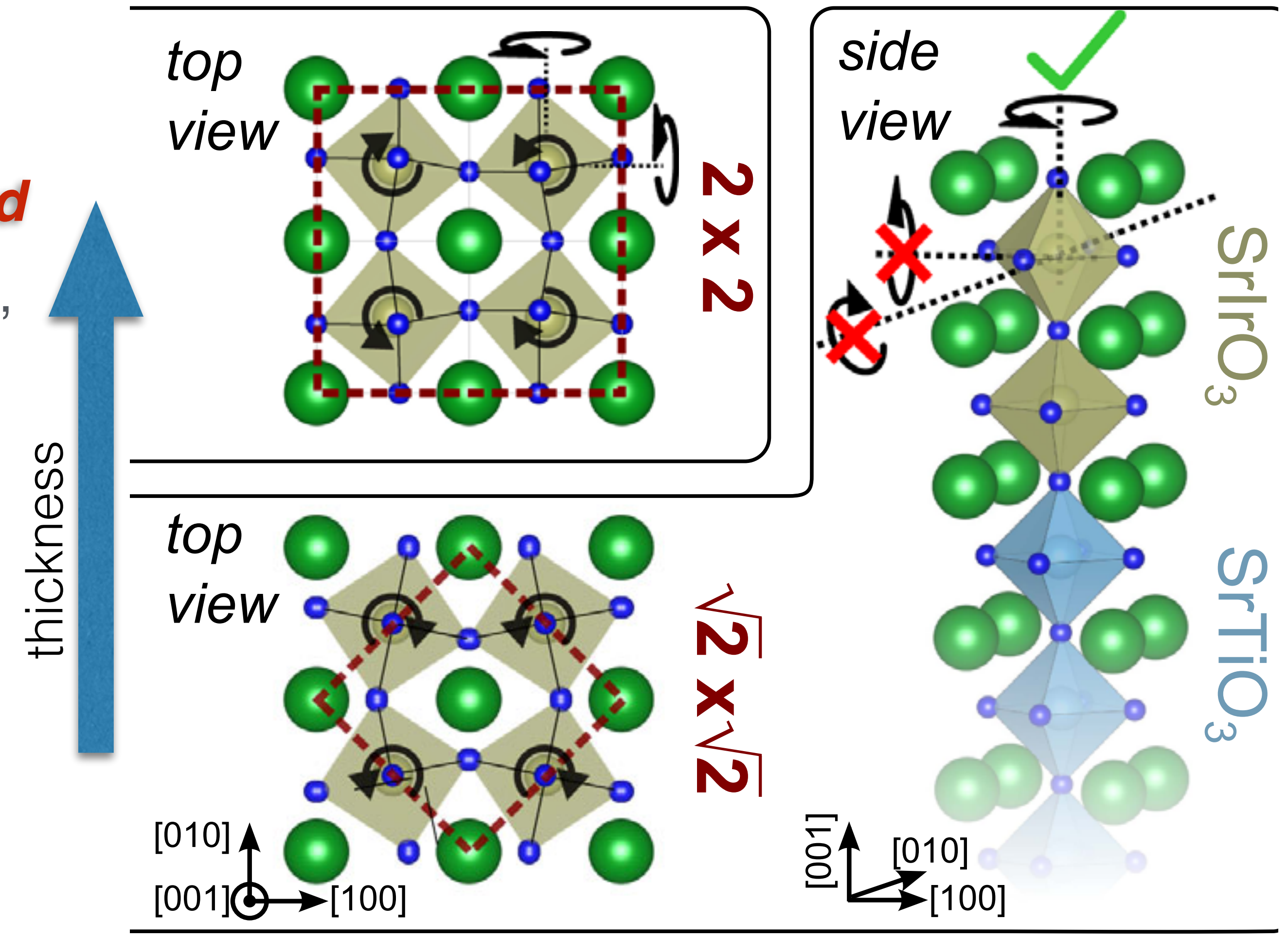

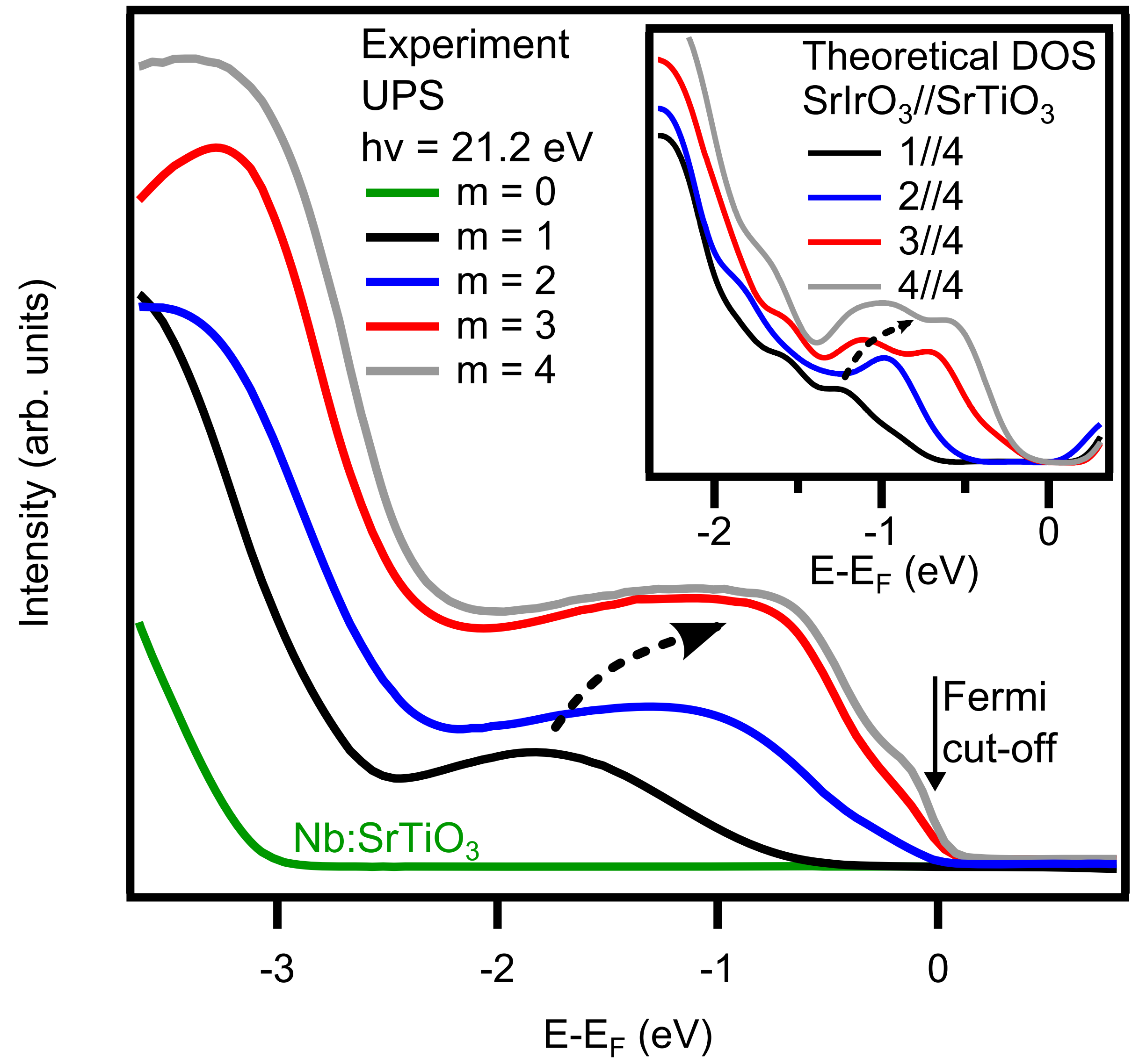

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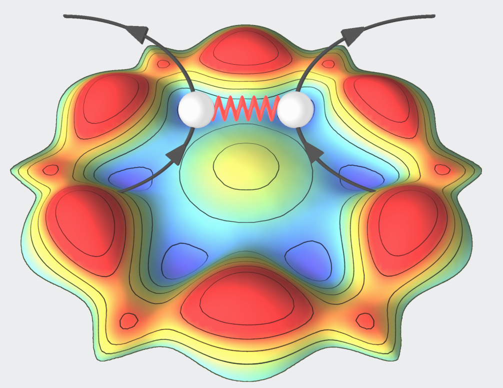

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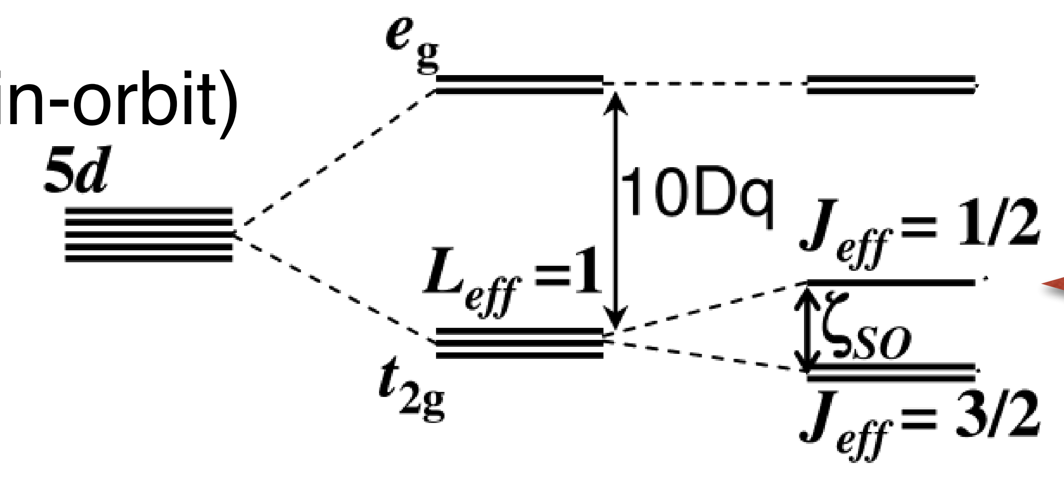

$SrIrO_3$

half-filled

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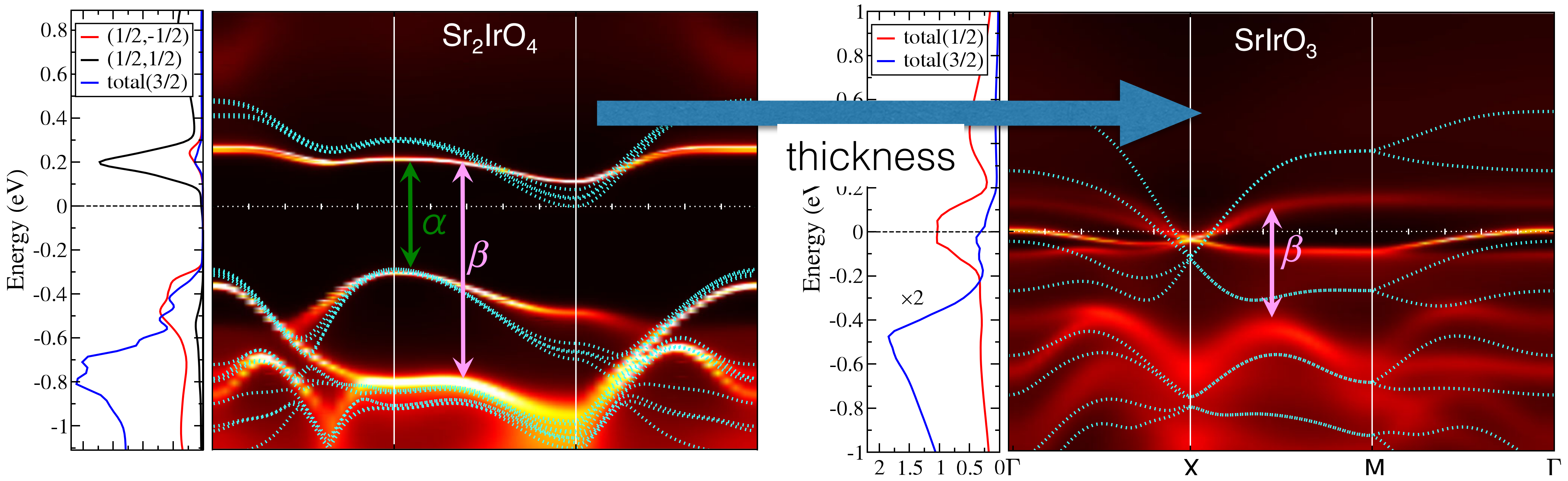

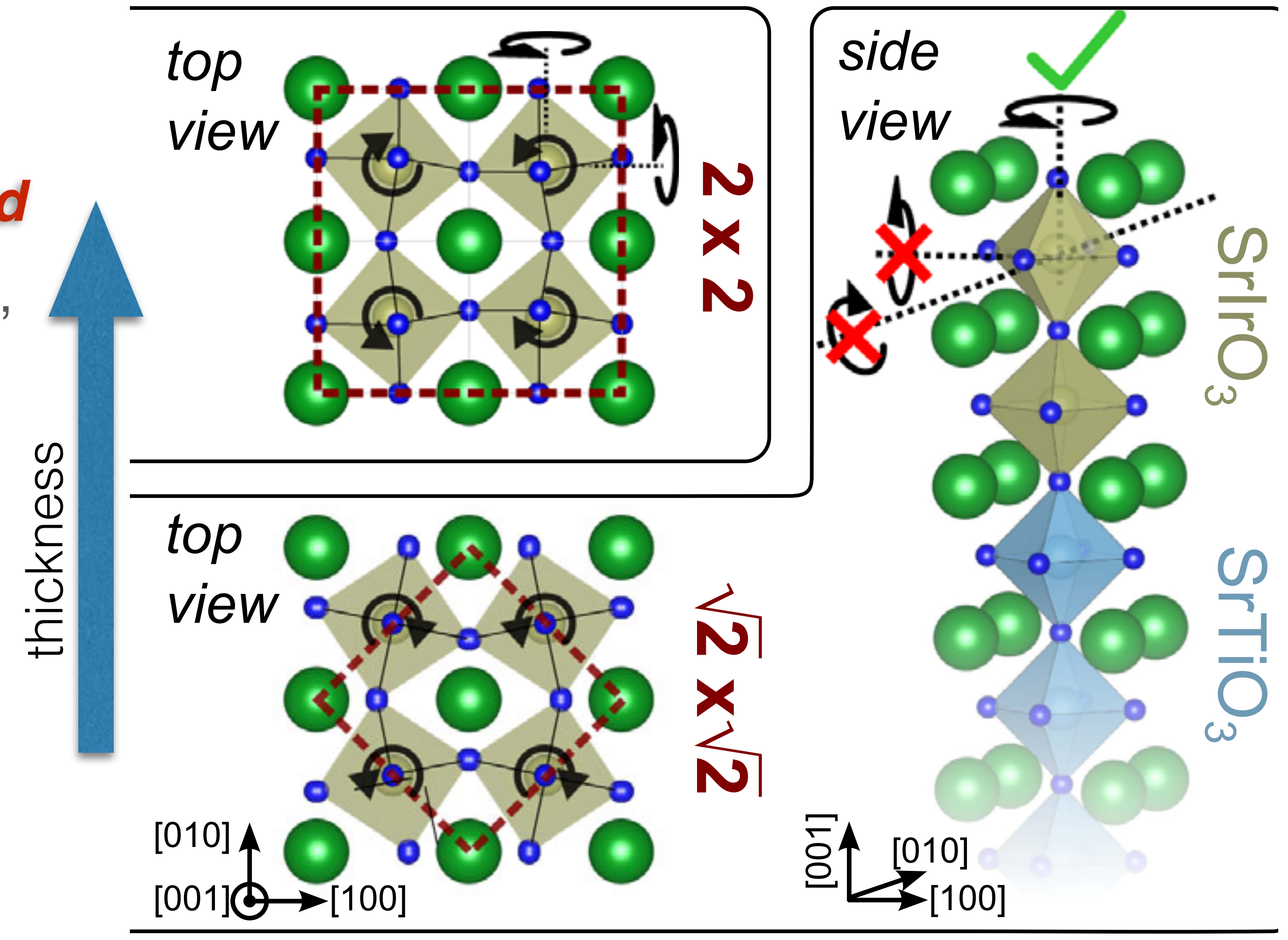

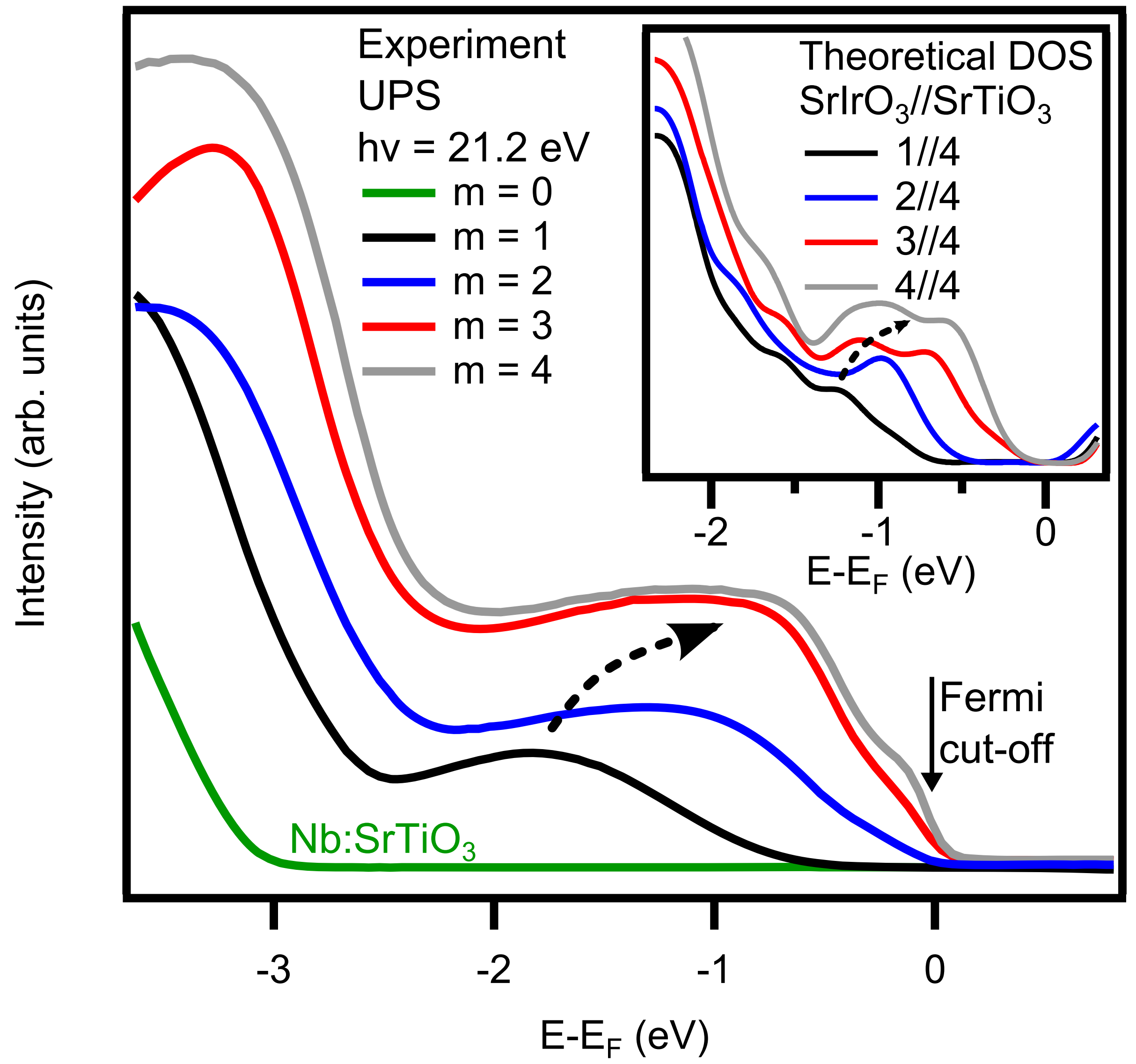

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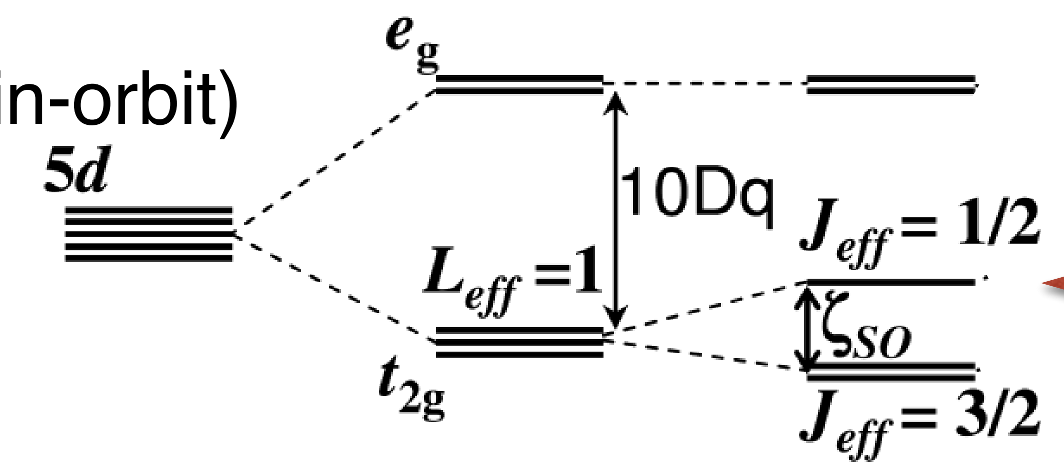

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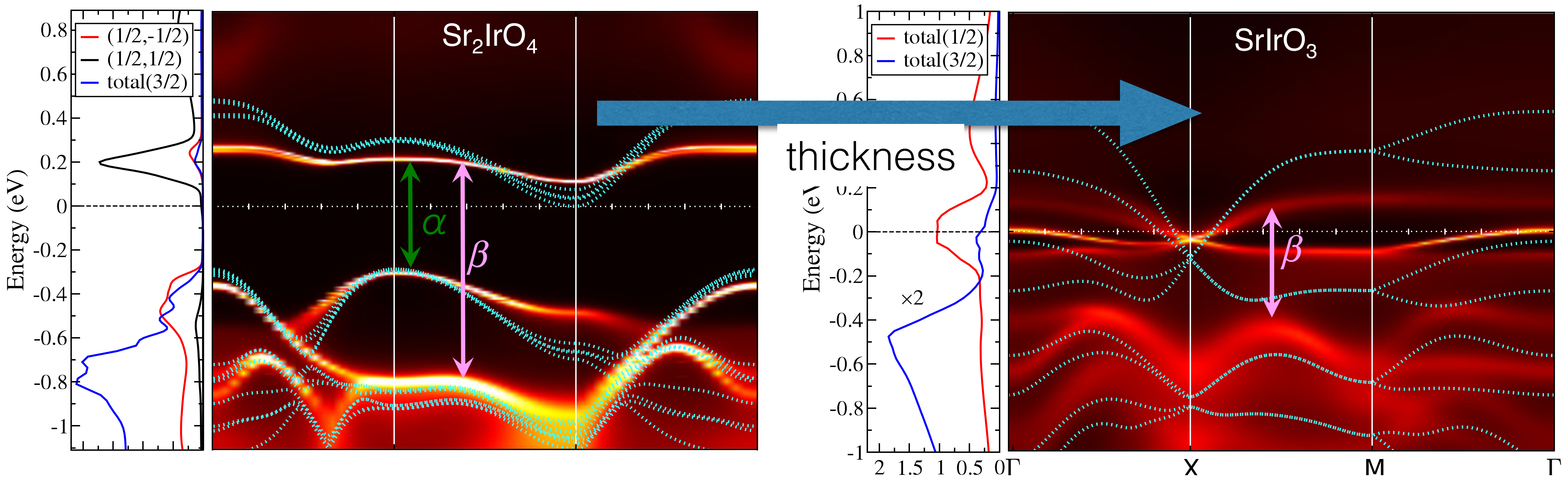

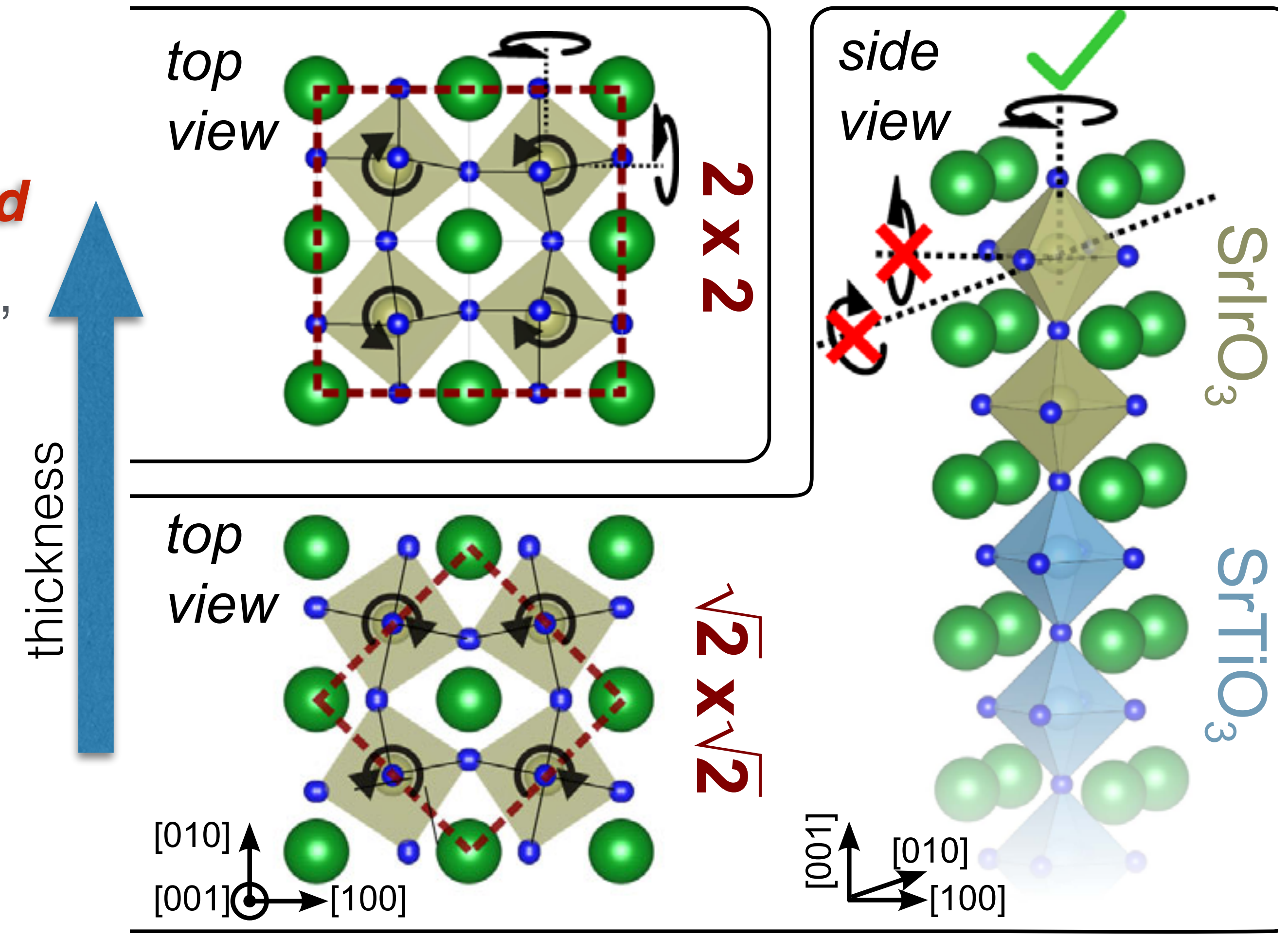

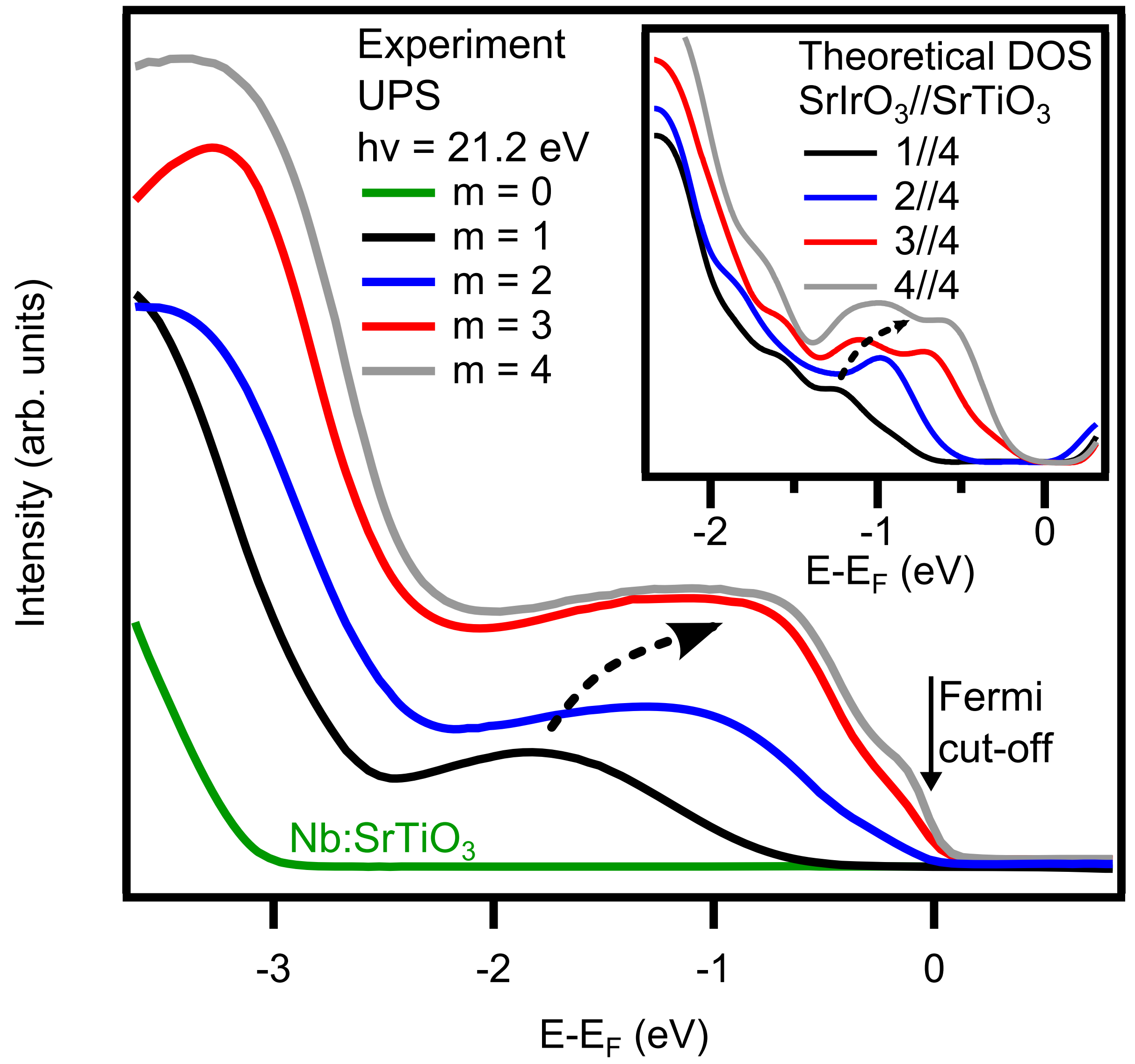

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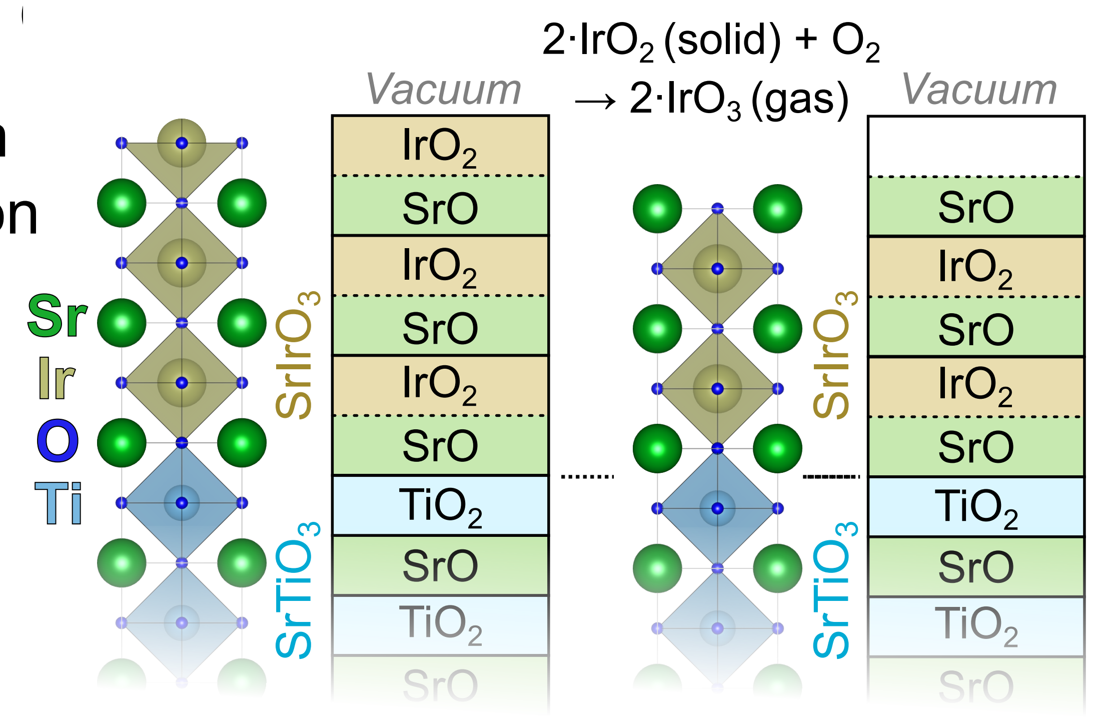
Termination conservation



Termination conversion

confirmed by DFT+U calculations (Domenico Di Sante)

P. Schütz, *et al.* submitted

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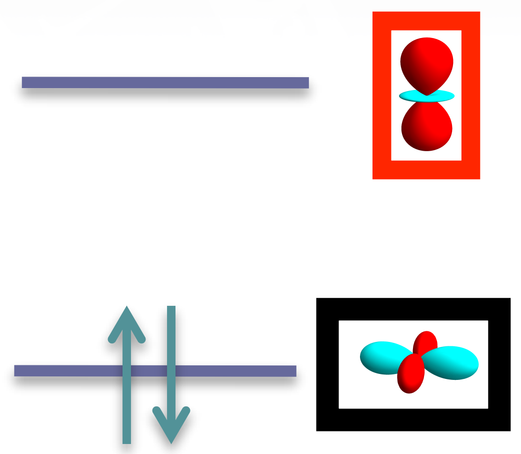
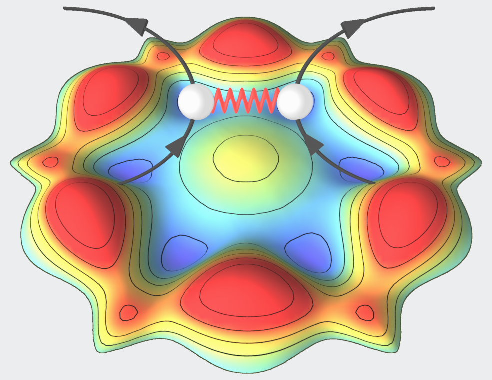
when do many-body effect go in the opposite direction?



- in nickel heterostructures: when the *d*-shell gets closer to d^8
- Hund’s tendecy to high-spin triplet Mott insulator in the e_g doublet



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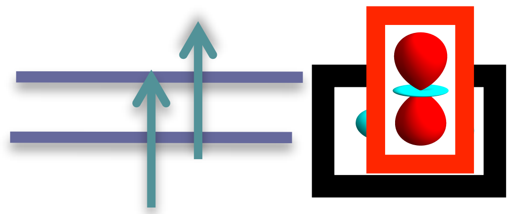

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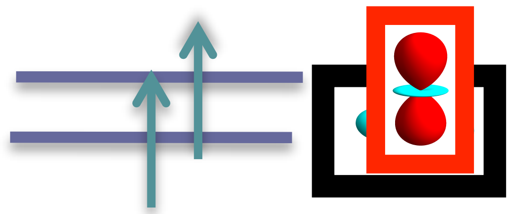

- HgTe (BHZ model) A. Bernevig, *et al.* Science (2006)
- Two orbitals (s p) and spin 1/2
- Time-reversal
- U(1)$_{\text{spin}}$ symmetry

$$\mathbf{H}_{4\times4}(\mathbf{k}) = \left(\begin{array}{c:c} \hat{h}_0(\mathbf{k}) & \uparrow\downarrow \\ \hdashline \downarrow\uparrow & \hat{h}_0^*(-\mathbf{k}) \end{array}\right)$$

Pauli matrices in orbital space

$$\hat{h}_0(\mathbf{k}) = \vec{d}(\mathbf{k}) \cdot \vec{\tau}$$

$$\vec{d}(\mathbf{k}) = \begin{pmatrix} \lambda \sin k_x \\ \lambda \sin k_y \\ M - \cos k_x - \cos k_y \end{pmatrix}$$

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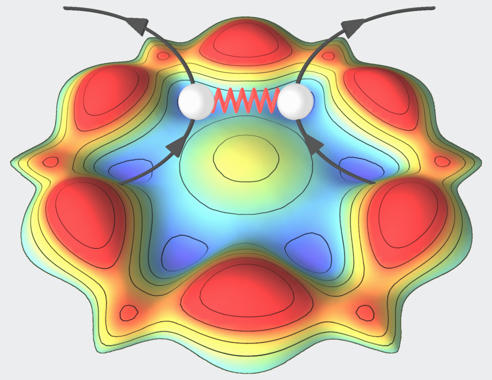

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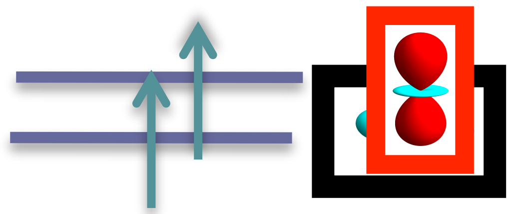

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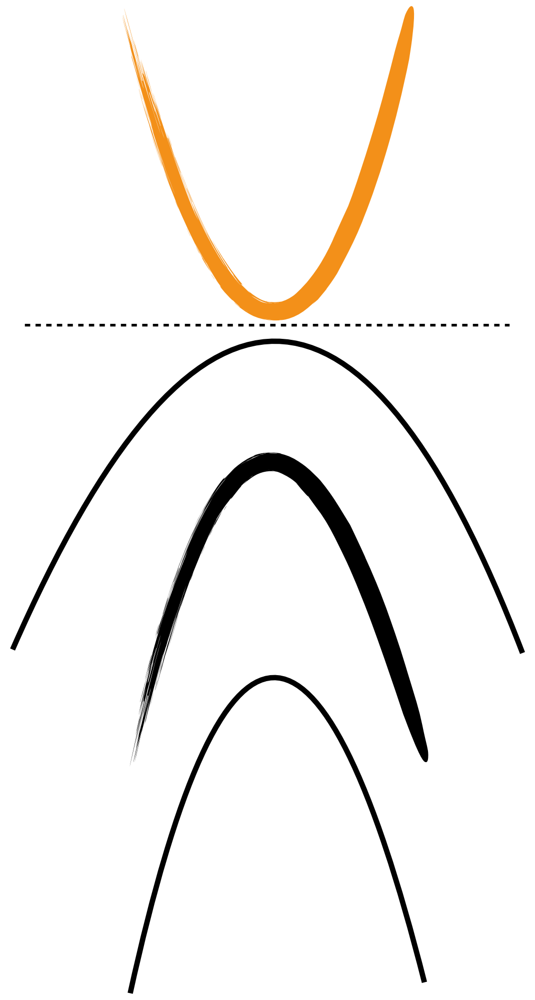
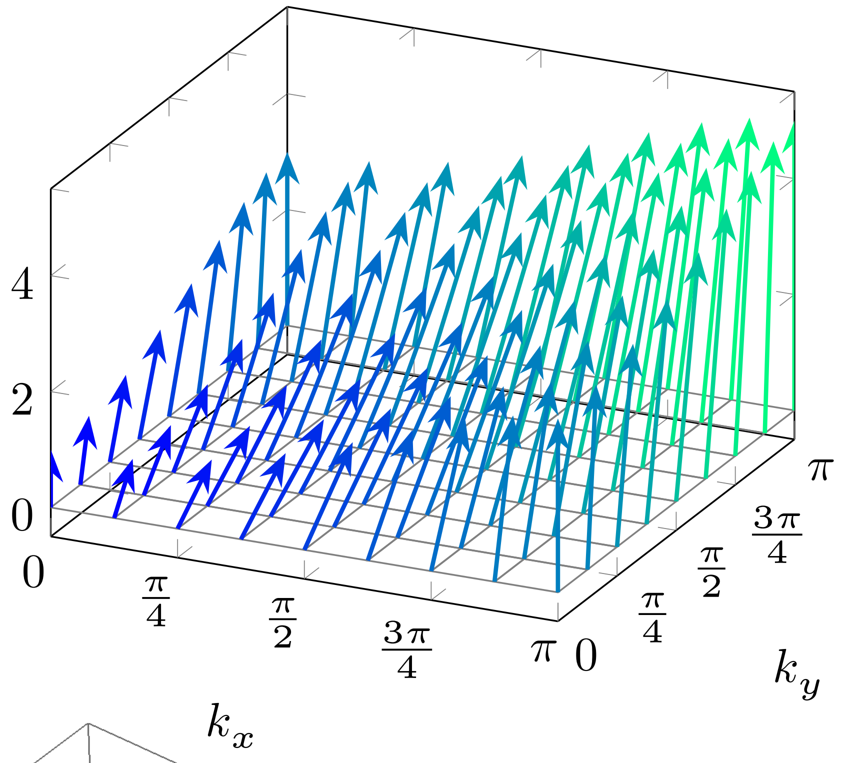
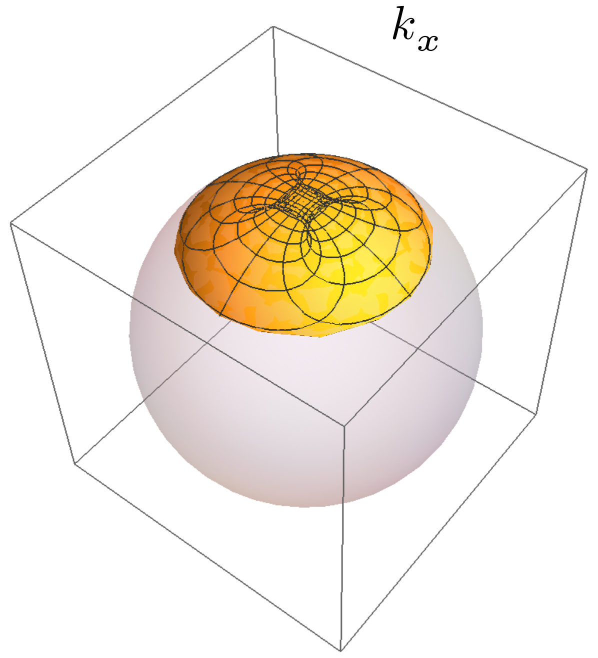
"non inverted"
M>2



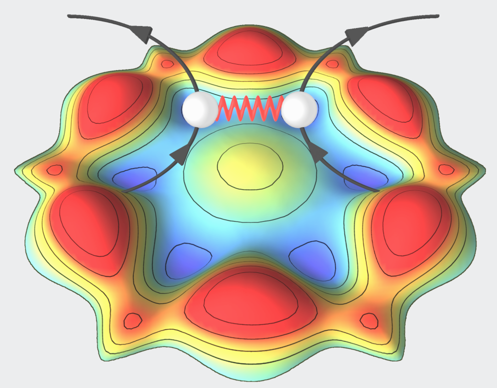


$\mathscr{C}_1$=0

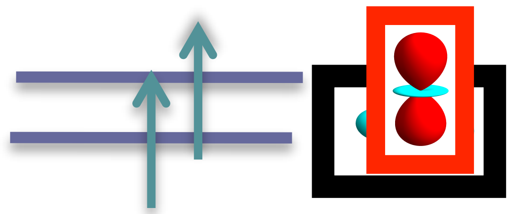


$$\vec{d}(\mathbf{k}) = \begin{pmatrix} \lambda \sin k_x \\ \lambda \sin k_y \\ M - \cos k_x - \cos k_y \end{pmatrix}$$

when do many-body effect go in the opposite direction?



- in nickel heterostructures: when the *d*-shell gets closer to d⁸
- Hund's tendecy to high-spin triplet Mott insulator in the e_g doublet



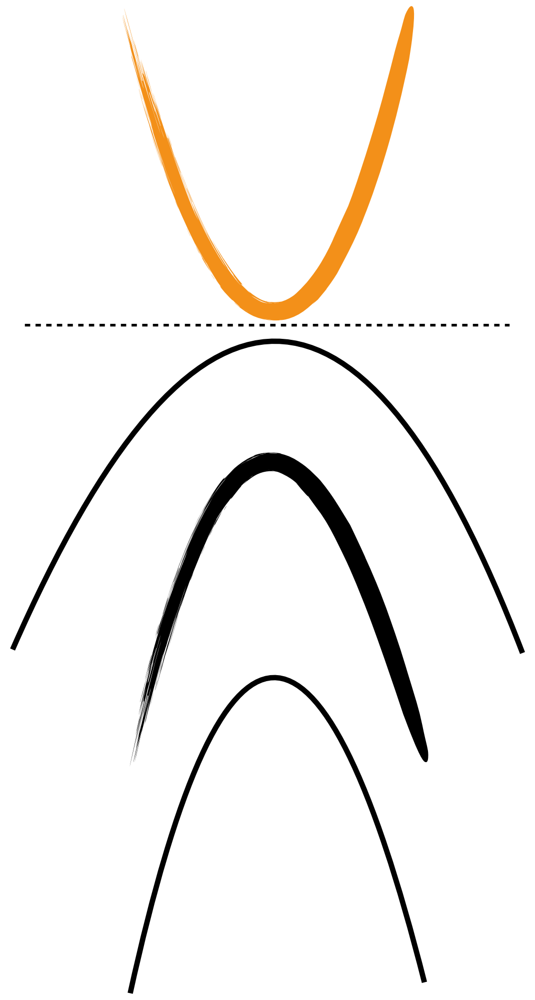
- HgTe (BHZ model) A. Bernevig, *et al.* Science (2006)
- Two orbitals (s p) and spin 1/2
- Time-reversal
- U(1)$_{\text{spin}}$ symmetry

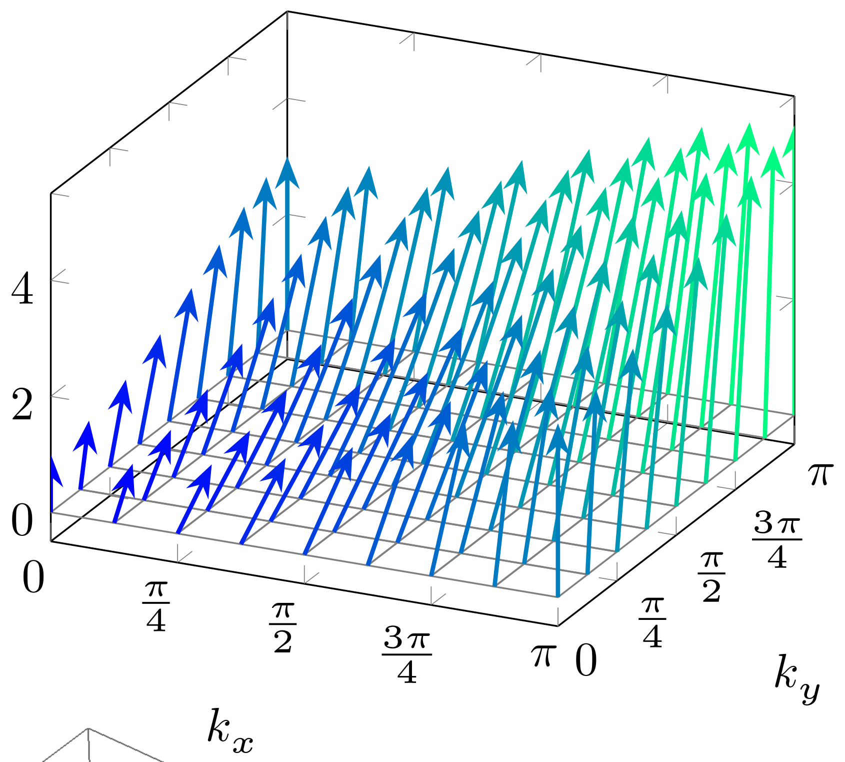
$$\mathbf{H}_{4\times4}(\mathbf{k}) = \left(\begin{array}{c:c} \hat{h}_0(\mathbf{k}) & \uparrow\downarrow \\ \hdashline \downarrow\uparrow & \hat{h}_0^*(-\mathbf{k}) \end{array}\right)$$

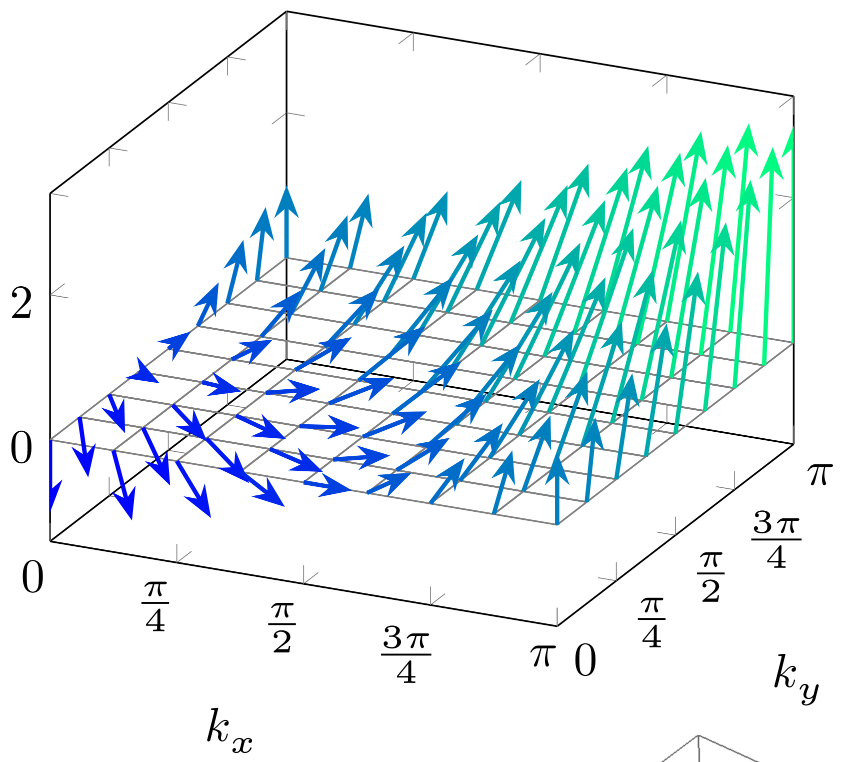
Pauli matrices in orbital space

$$\hat{h}_0(\mathbf{k}) = \vec{d}(\mathbf{k}) \cdot \vec{\tau}$$

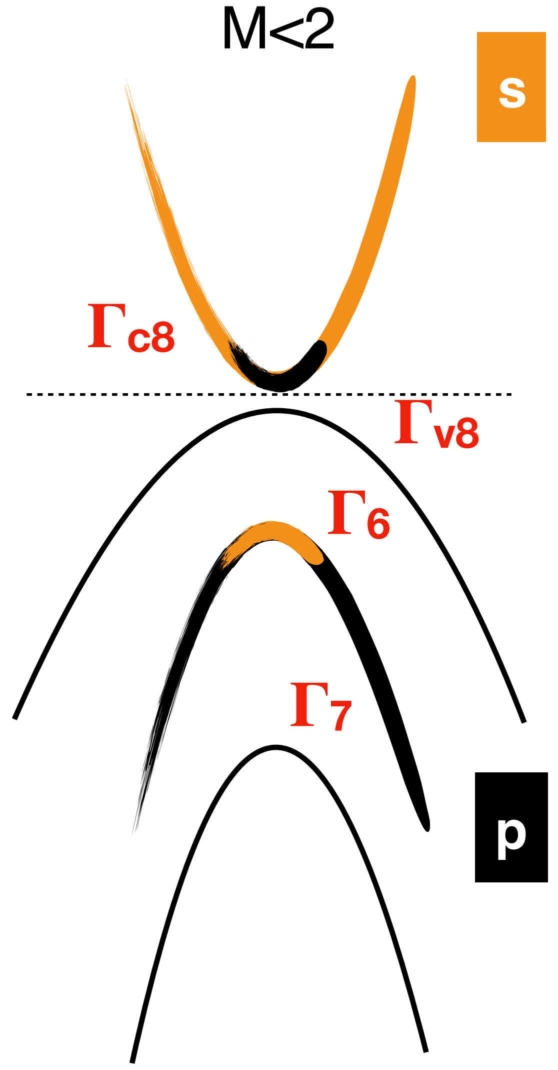
"non inverted"
M>2



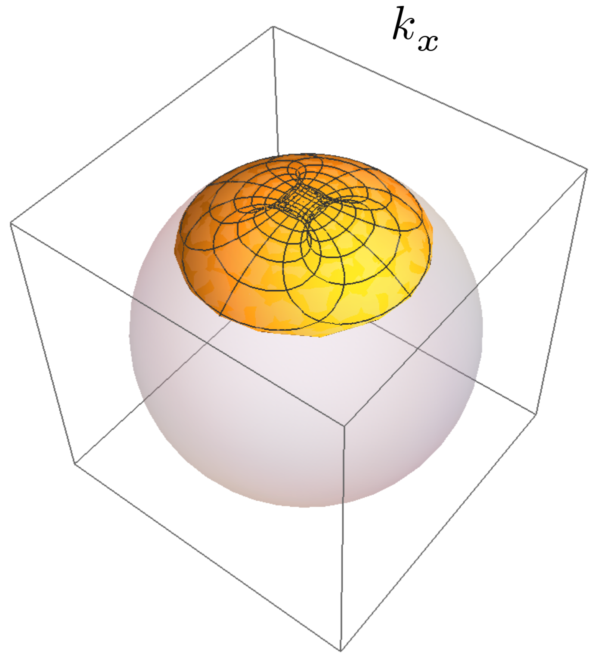




"inverted"
M<2



$\mathscr{C}_1$=0



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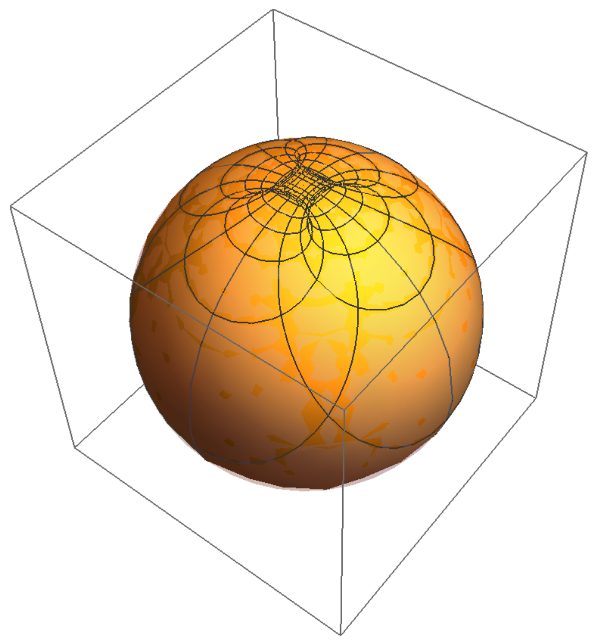
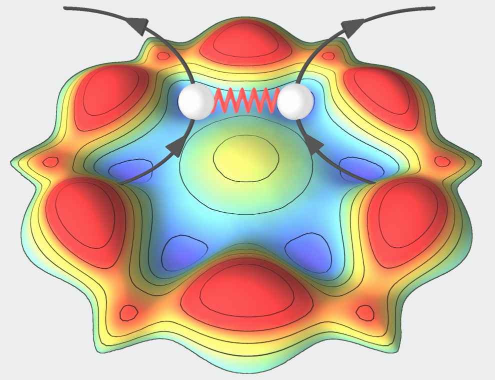


$\mathscr{C}_1$=1

BHZ-Hubbard model



- orbital structure of interaction for the BHZ + Hubbard U, Hund J
- simplest local interaction term
  [see A. Georges, L. de' Medici and J. Mravlje, Annu. Rev. Condens. Matter Phys. (2013)]

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Y. Tada, *et al.* PRB (2012)
T. Yoshida, *et al.* PRB (2012)
L. Wang, *et al.* EPL (2012)
J. Budich, *et al.* PRB (2012)
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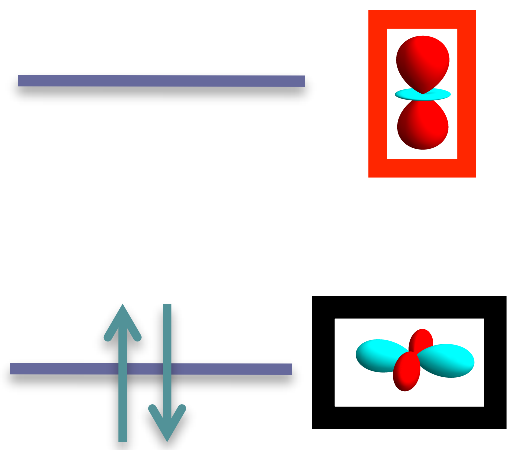
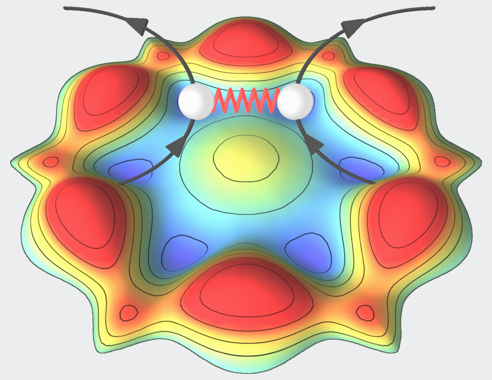
$$\mathcal{H}_{\mathrm{int}}(\mathrm{i}) = (U - J)\frac{N_{\mathrm{i}}(N_{\mathrm{i}} - 1)}{2} - J\left(\frac{N_{\mathrm{i}}^2}{4} + S_{z\mathrm{i}}^2 - 2T_{z\mathrm{i}}^2\right)$$





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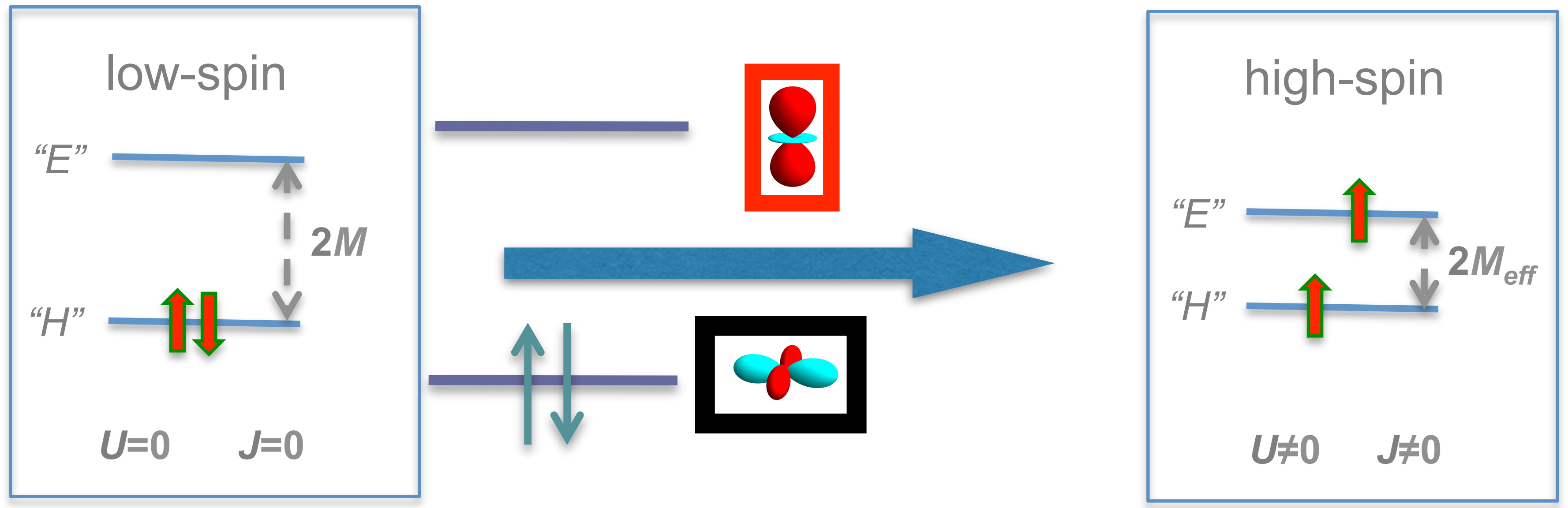

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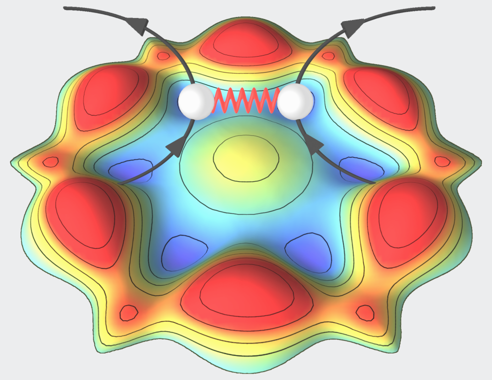

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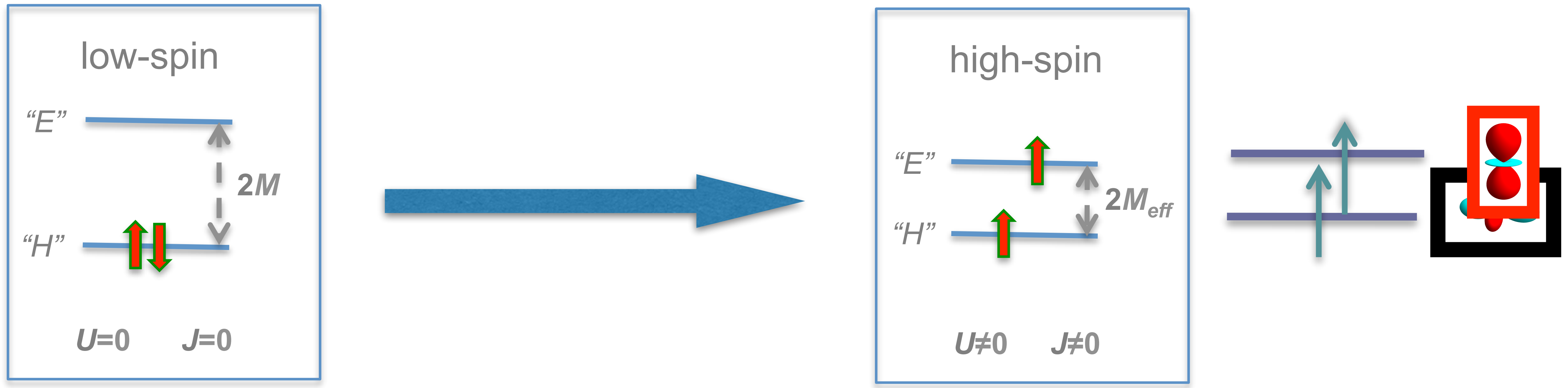

- Intra- + inter-orbital *J* (Hund) interaction

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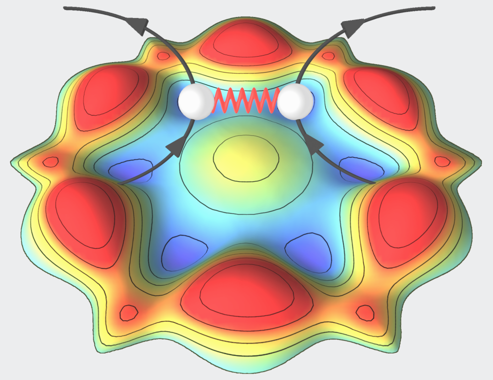
BHZ-Hubbard model



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Y. Tada, *et al.* PRB (2012)
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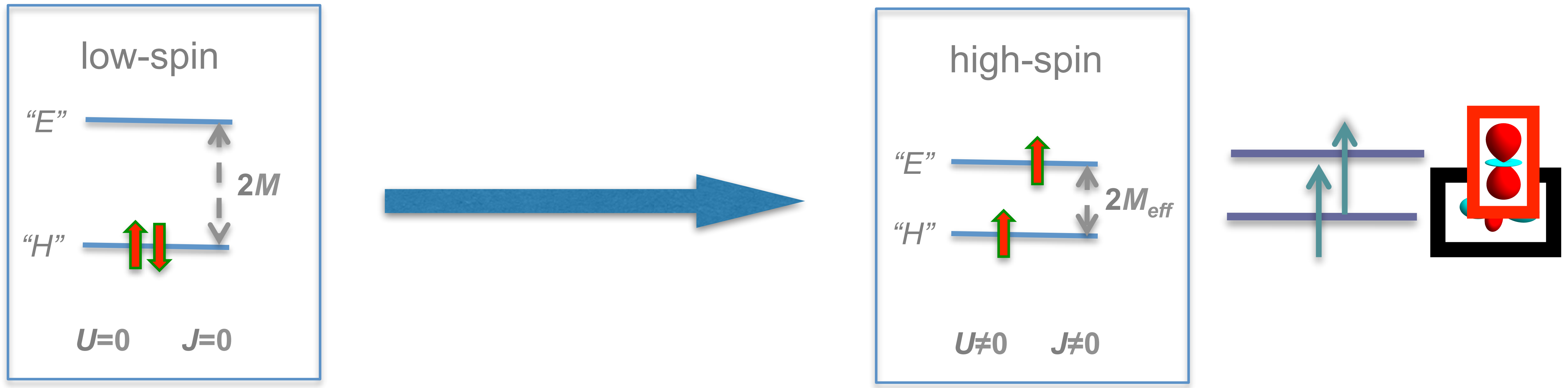

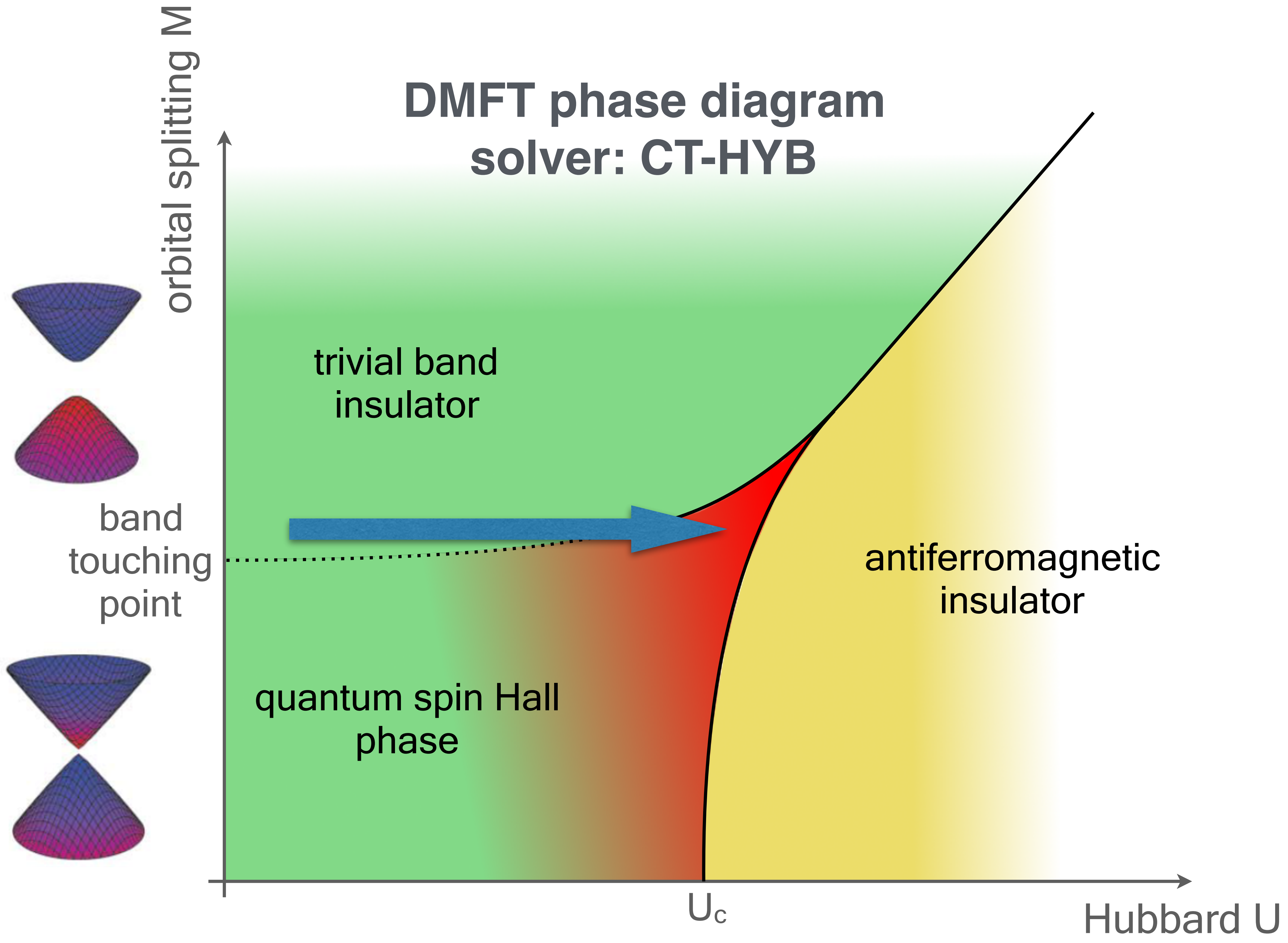

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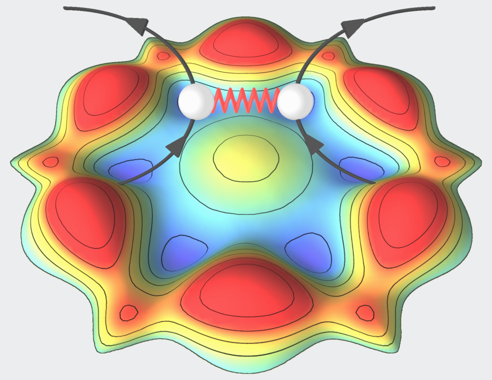
BHZ-Hubbard model



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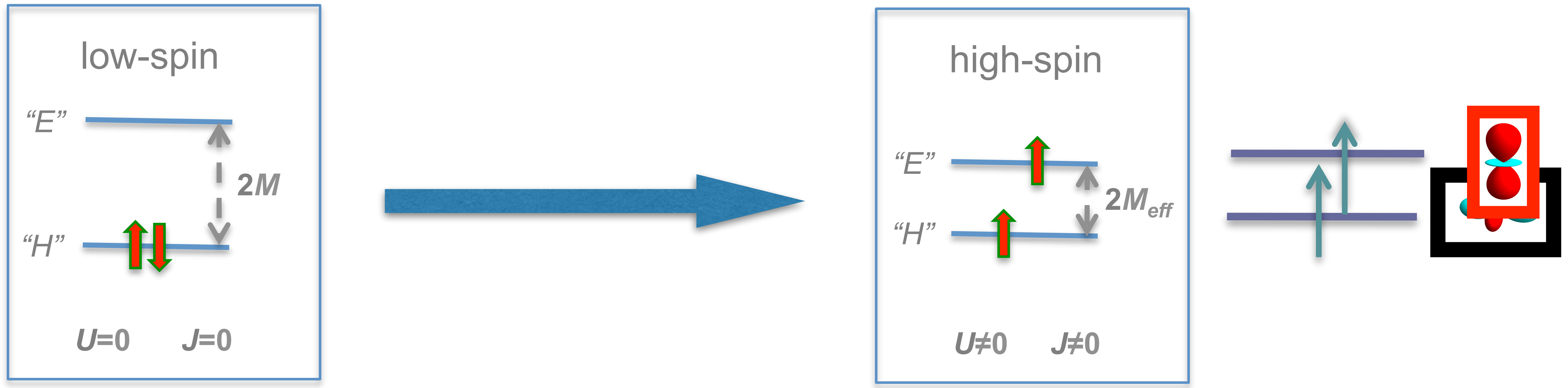

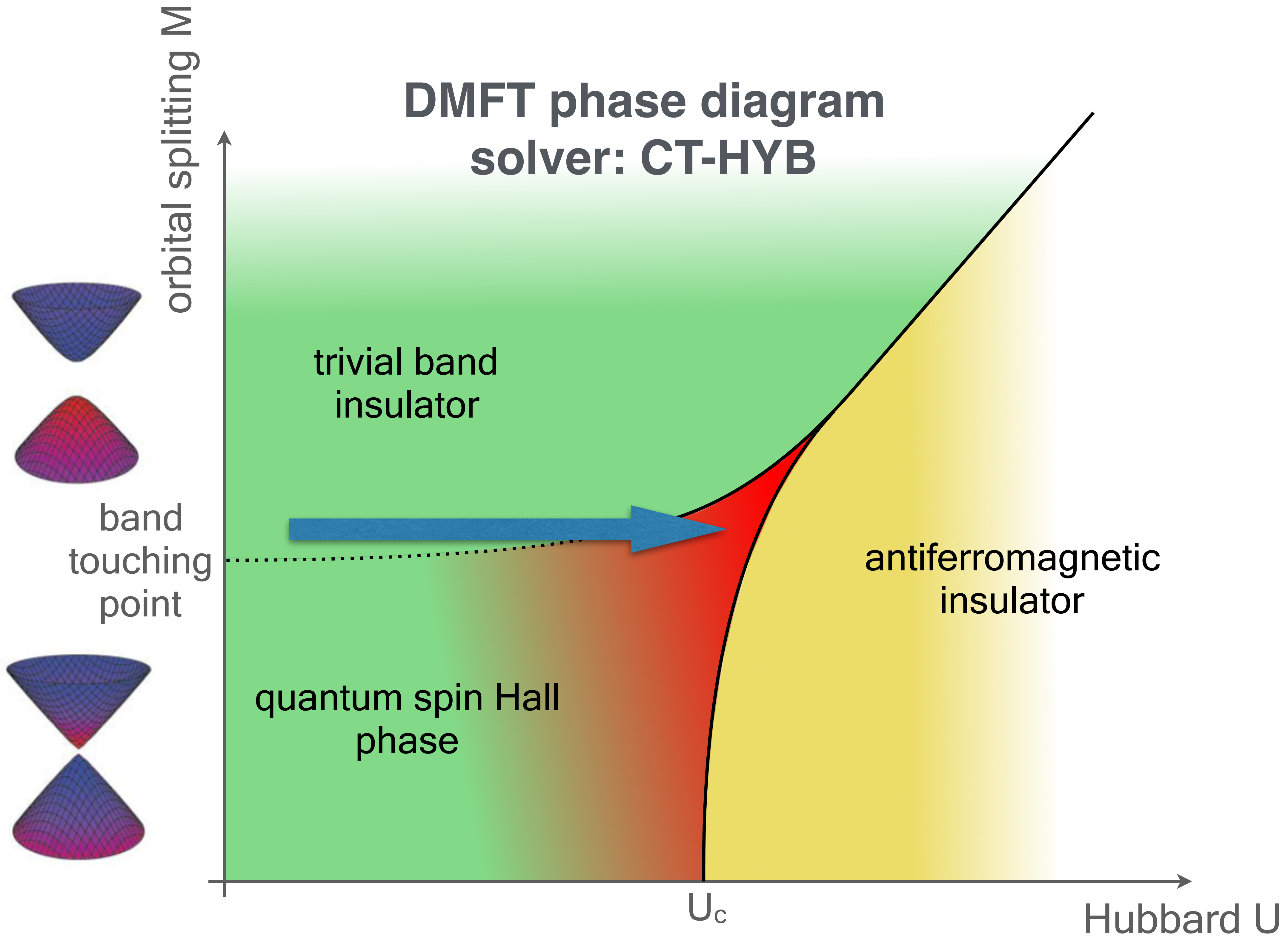

- Intra- + inter-orbital J (Hund) interaction

- U suppresses double occupancies $\Longrightarrow$ reduced effective orbital splitting $M_{\rm eff}$

- QSH extends at large-U and large-M, as a "precursor" of the high-spin phase

- …but there is more to that: see color coding in the phase diagram!

BHZ-Hubbard model

- where do the colors come from?

$$\mathcal{H}_{\mathrm{int}}(\mathrm{i}) = (U-J)\frac{N_{\mathrm{i}}(N_{\mathrm{i}}-1)}{2} - J\left(\frac{N_{\mathrm{i}}^2}{4} + S_{z\mathrm{i}}^2 - 2T_{z\mathrm{i}}^2\right)$$

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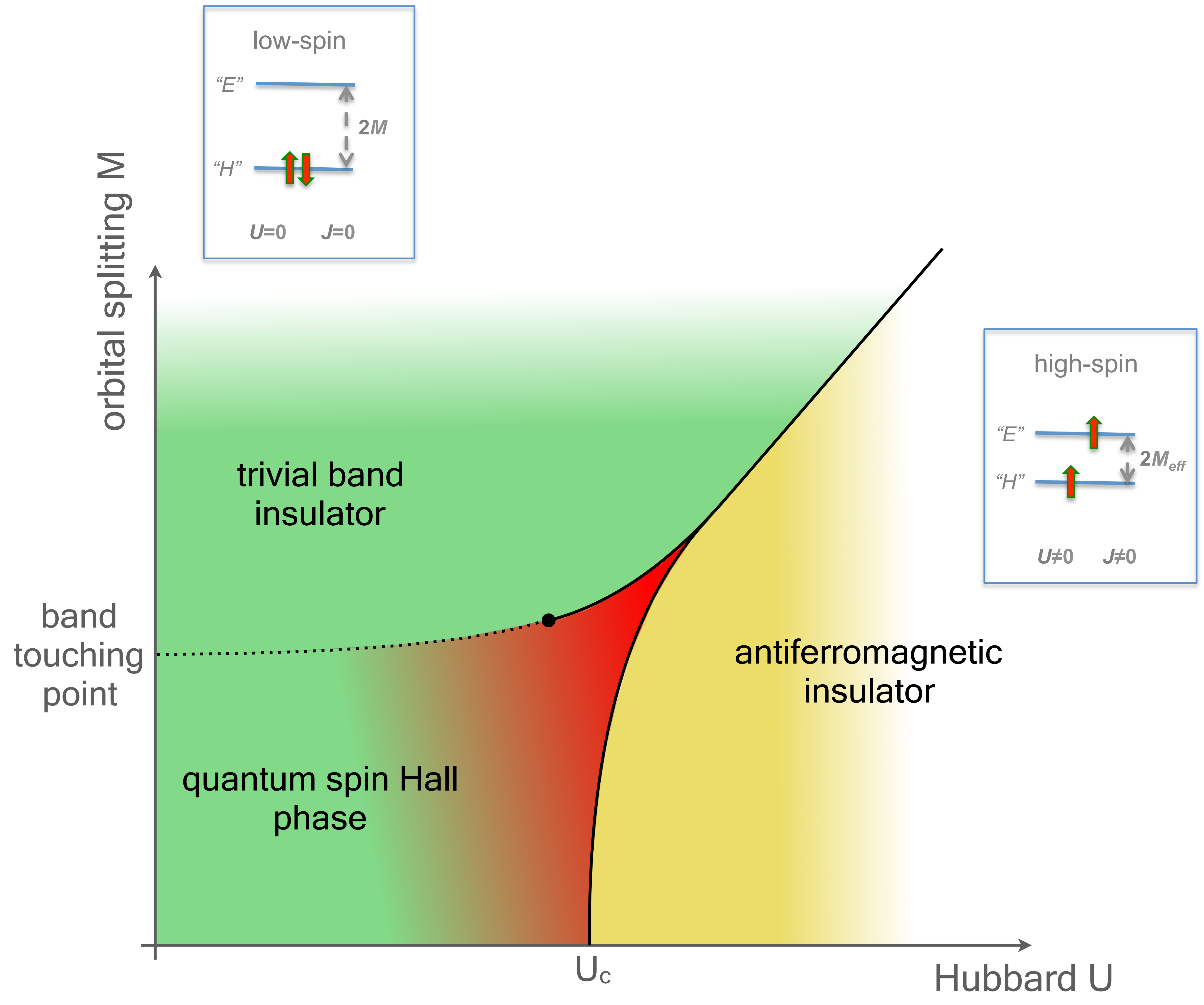
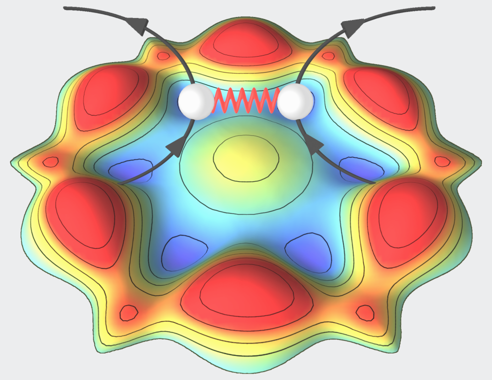


BHZ-Hubbard model



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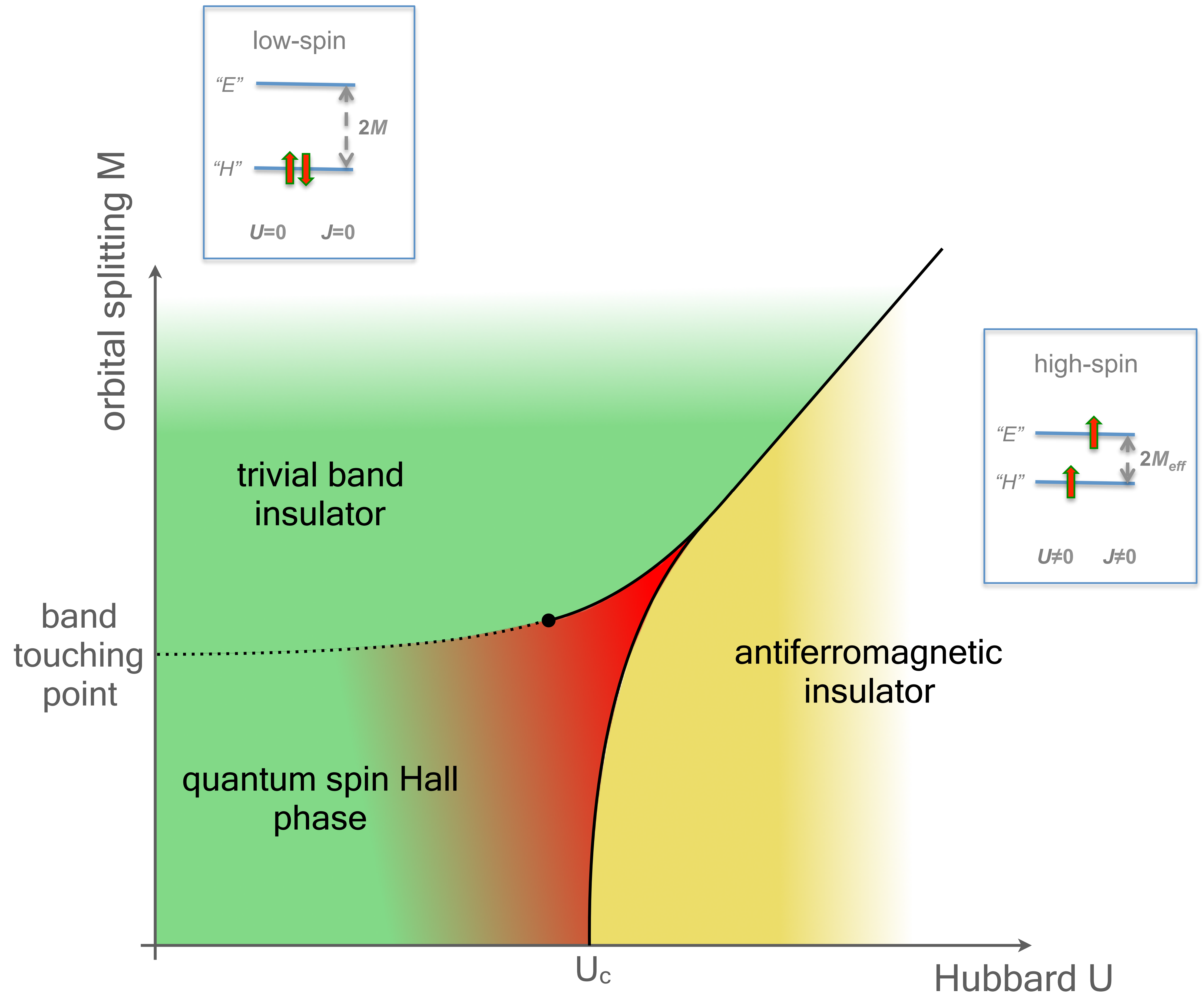
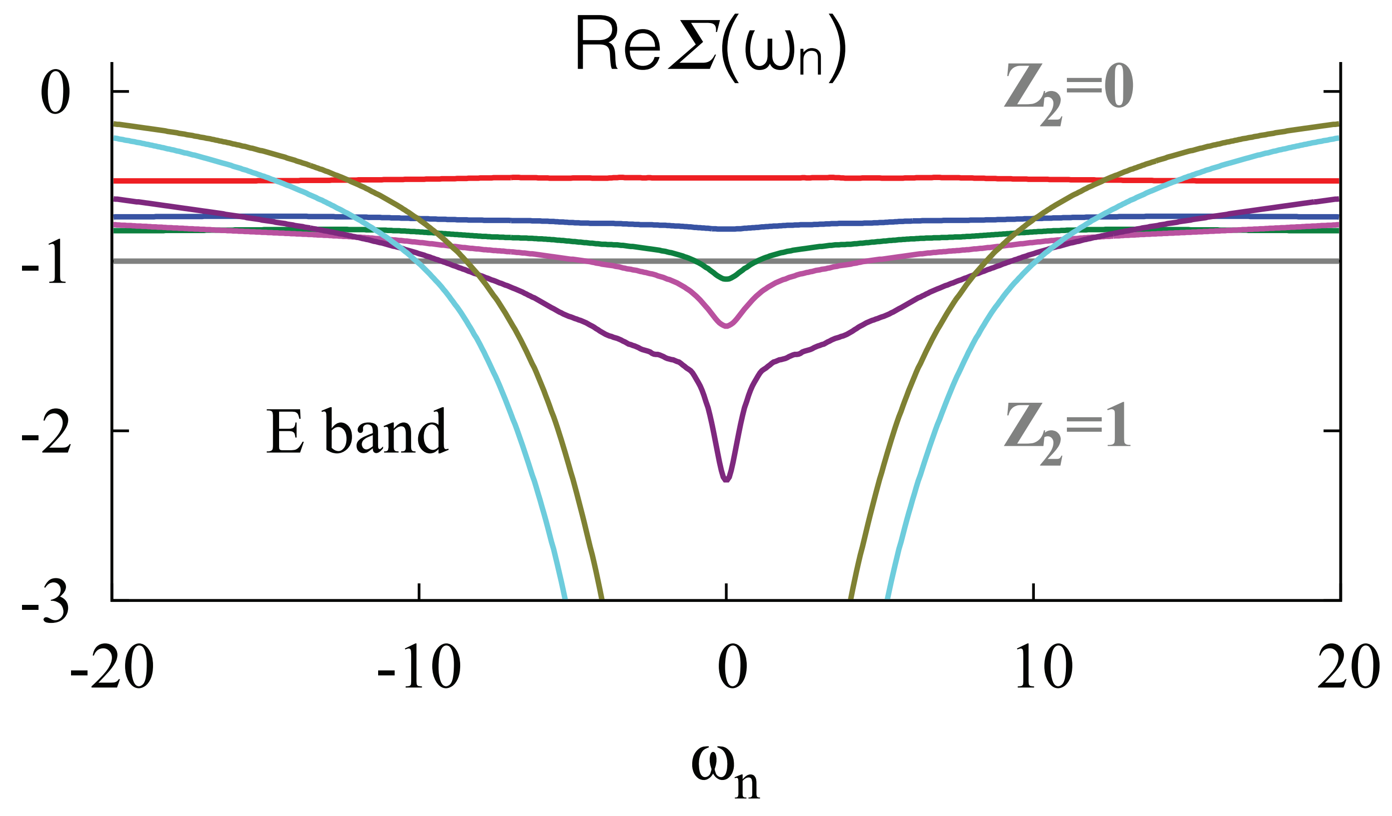


- distinction between flat "Hartree-Fock" and
- pronounced ω-structure of many-body nature



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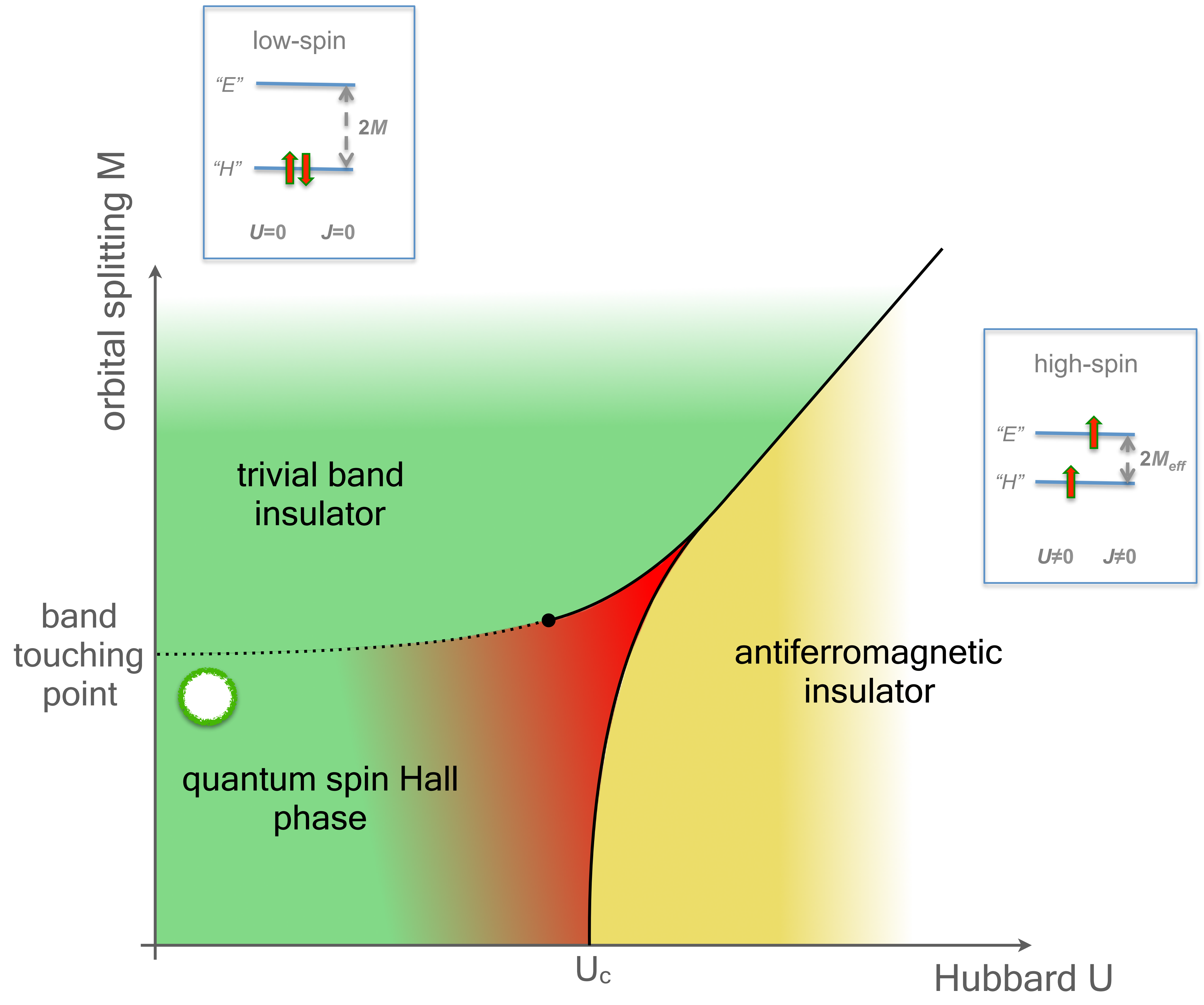

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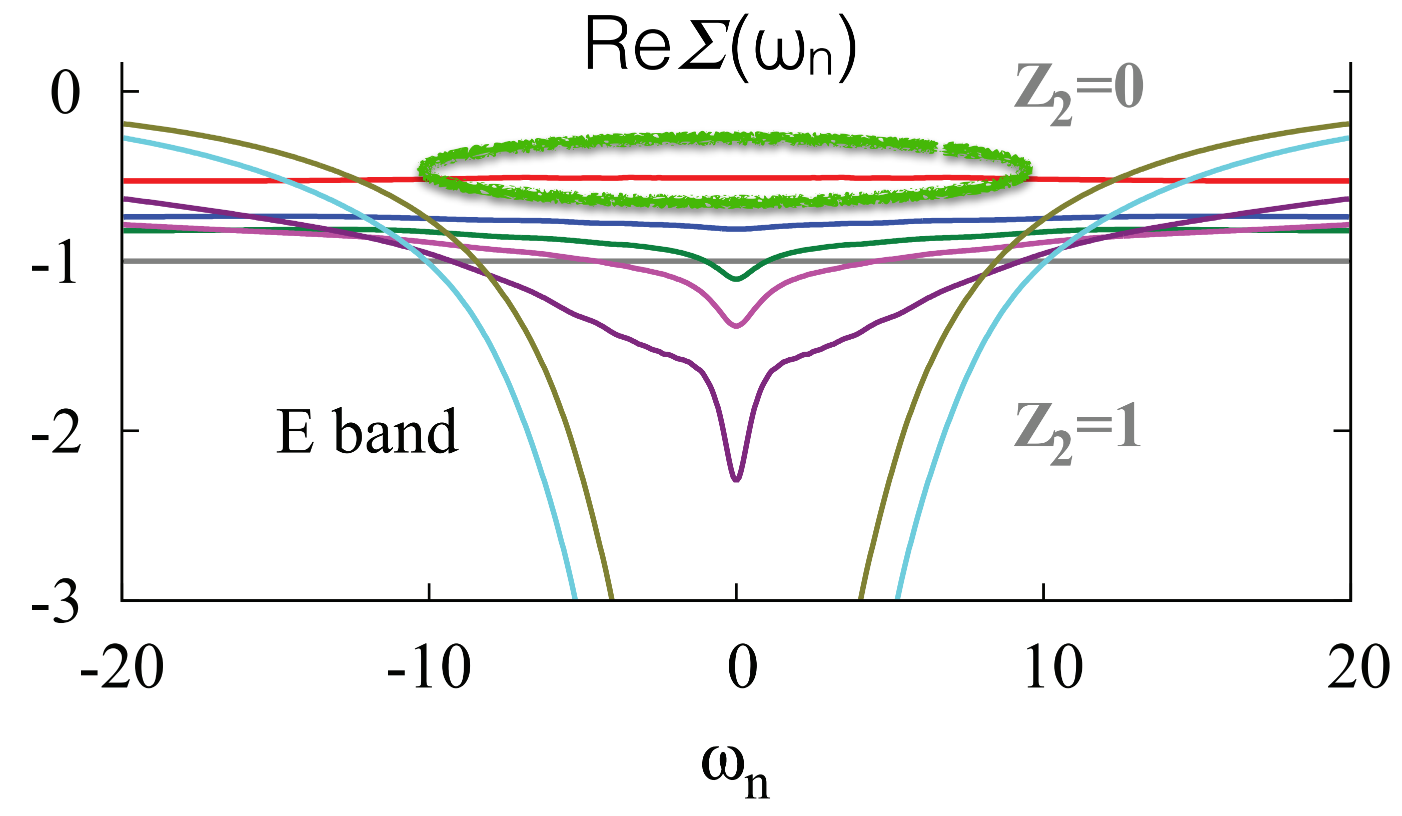

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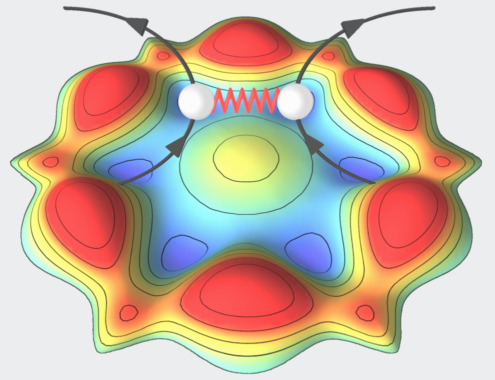

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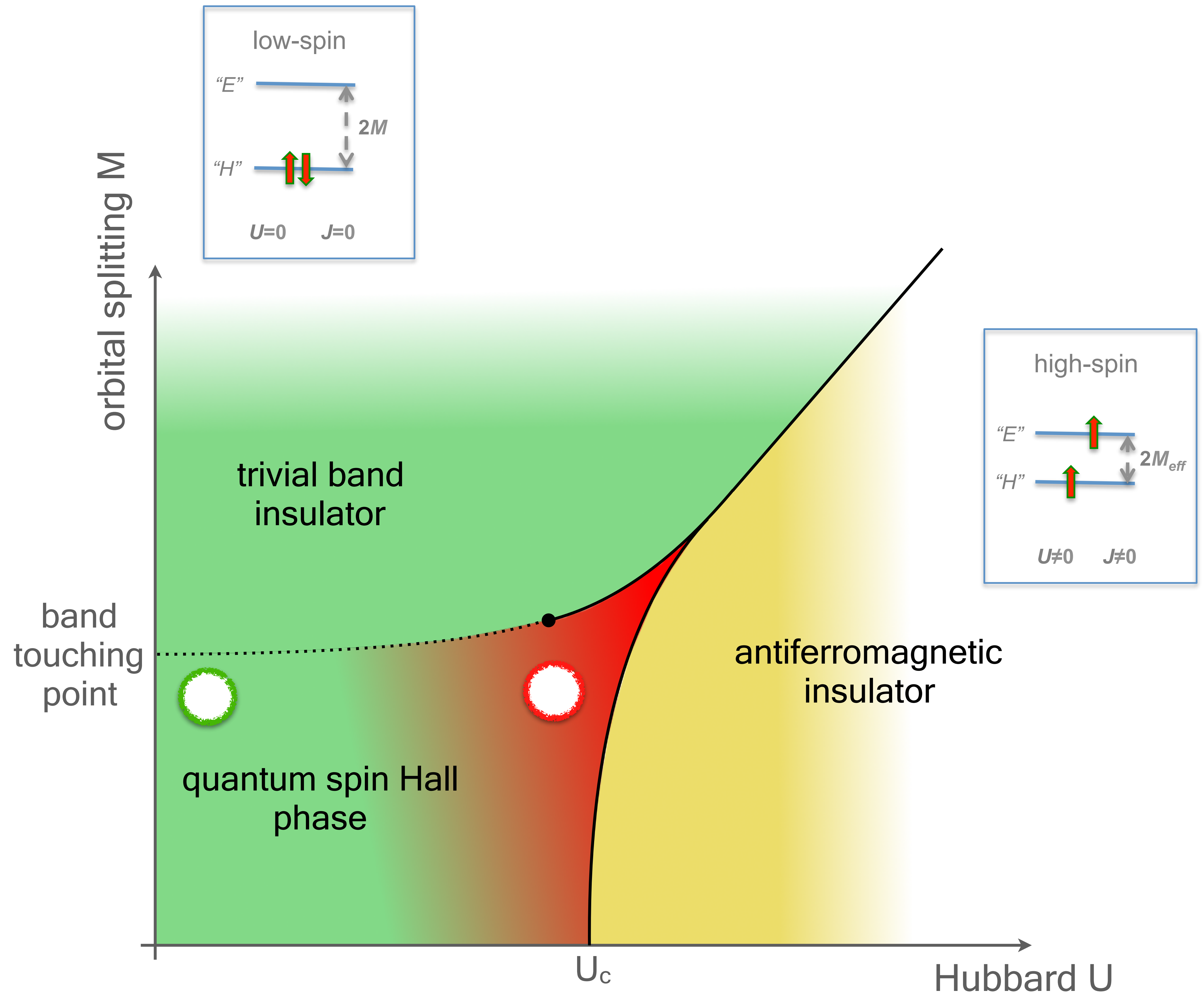

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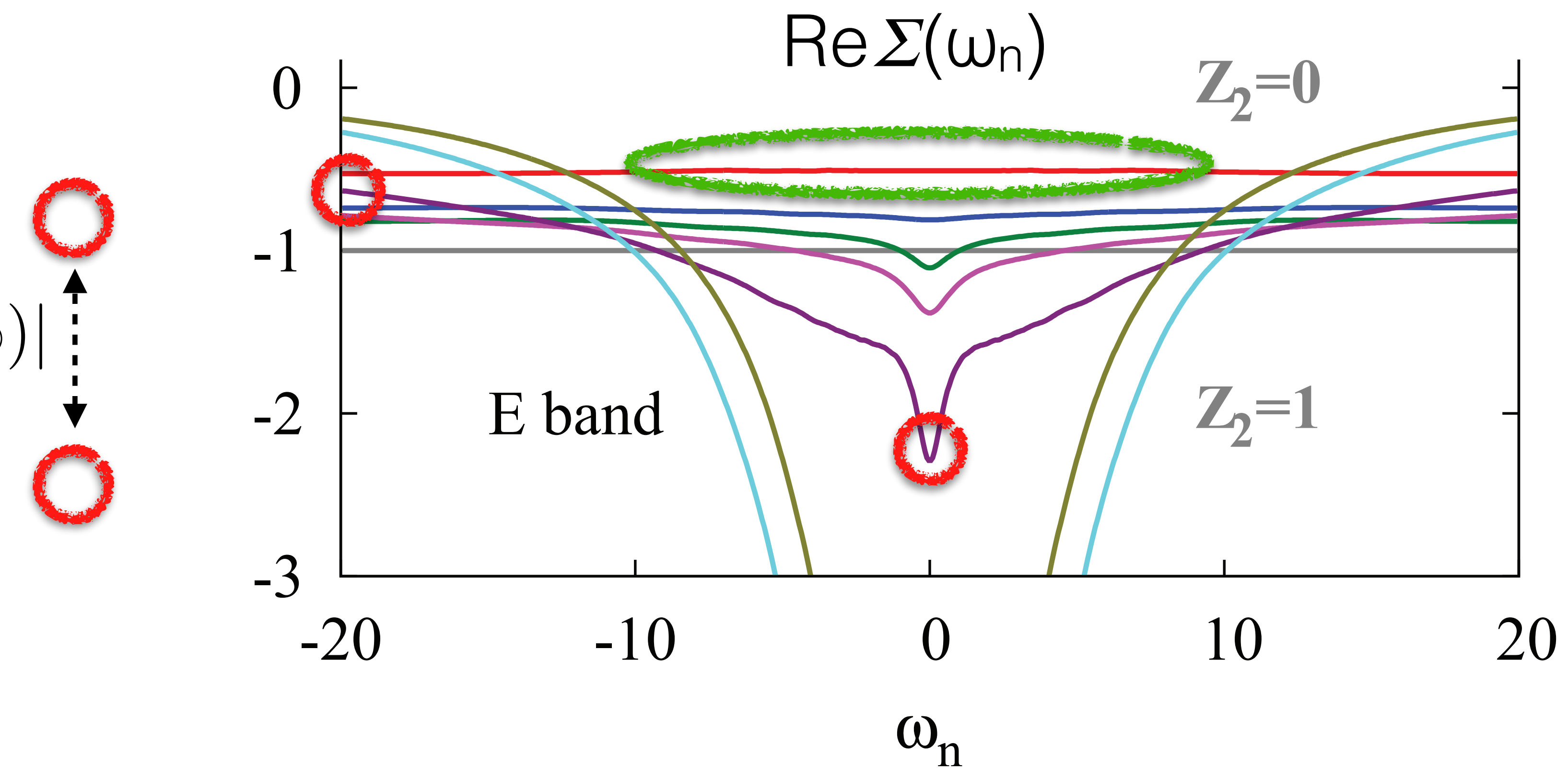
color scale:

$|\mathrm{Re}\Sigma(\omega\!=\!0) - \mathrm{Re}\Sigma(\omega\!=\!\infty)|$



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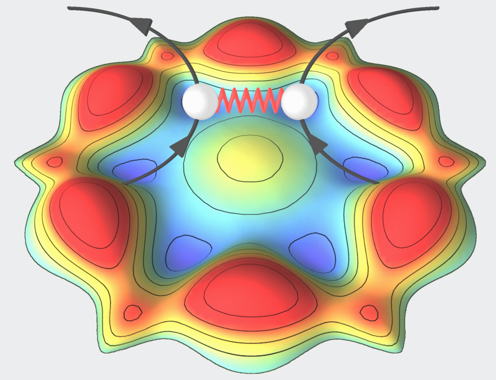

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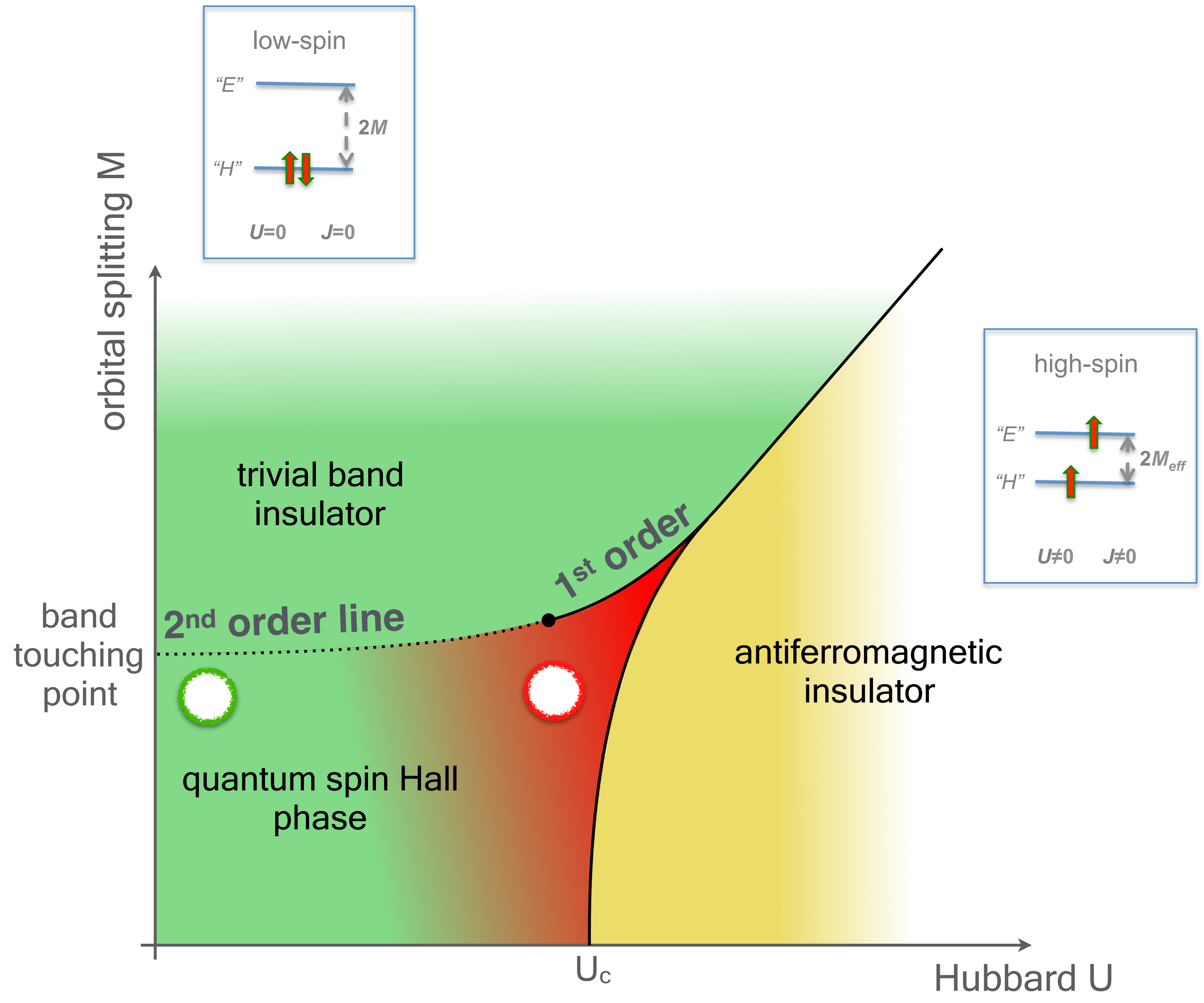

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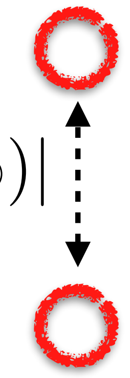
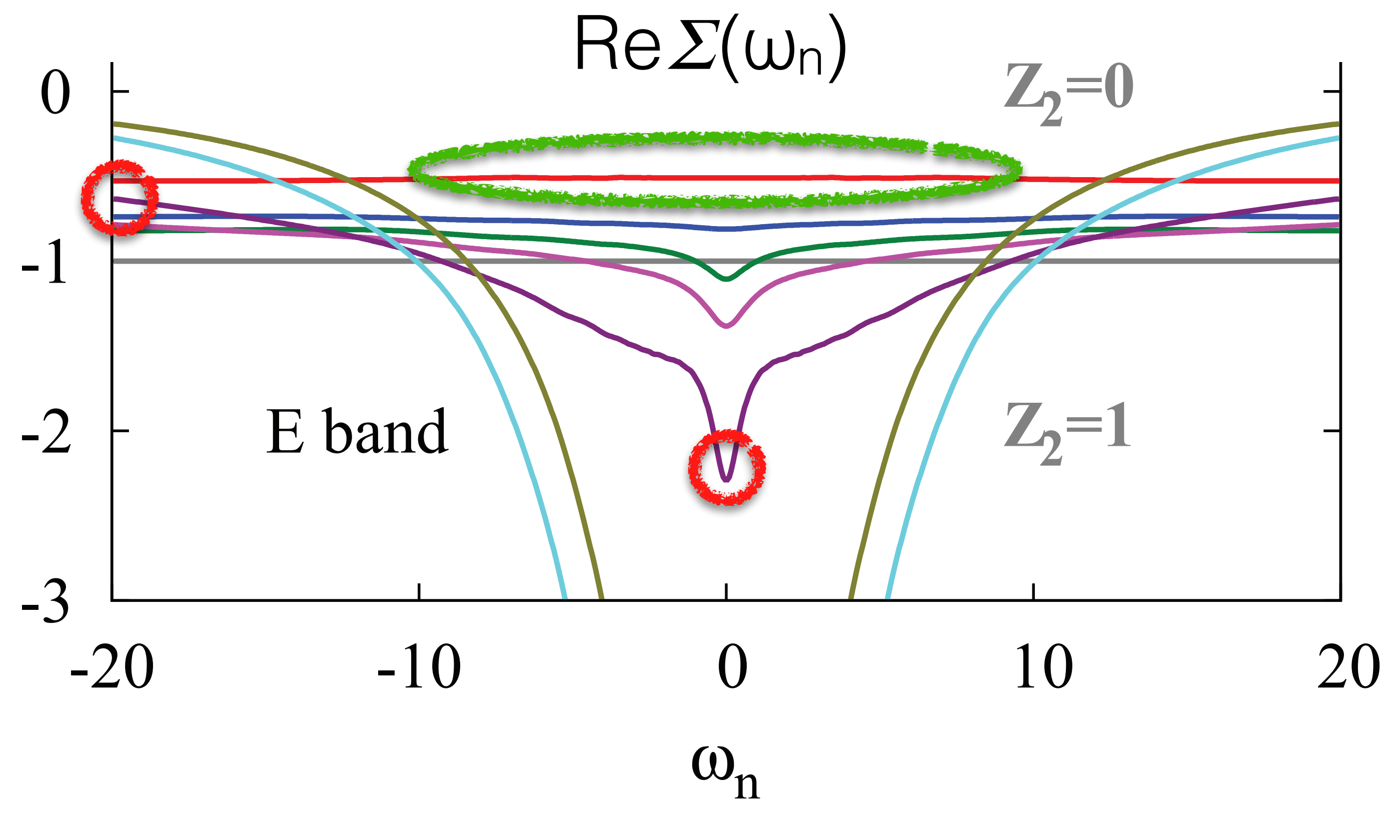


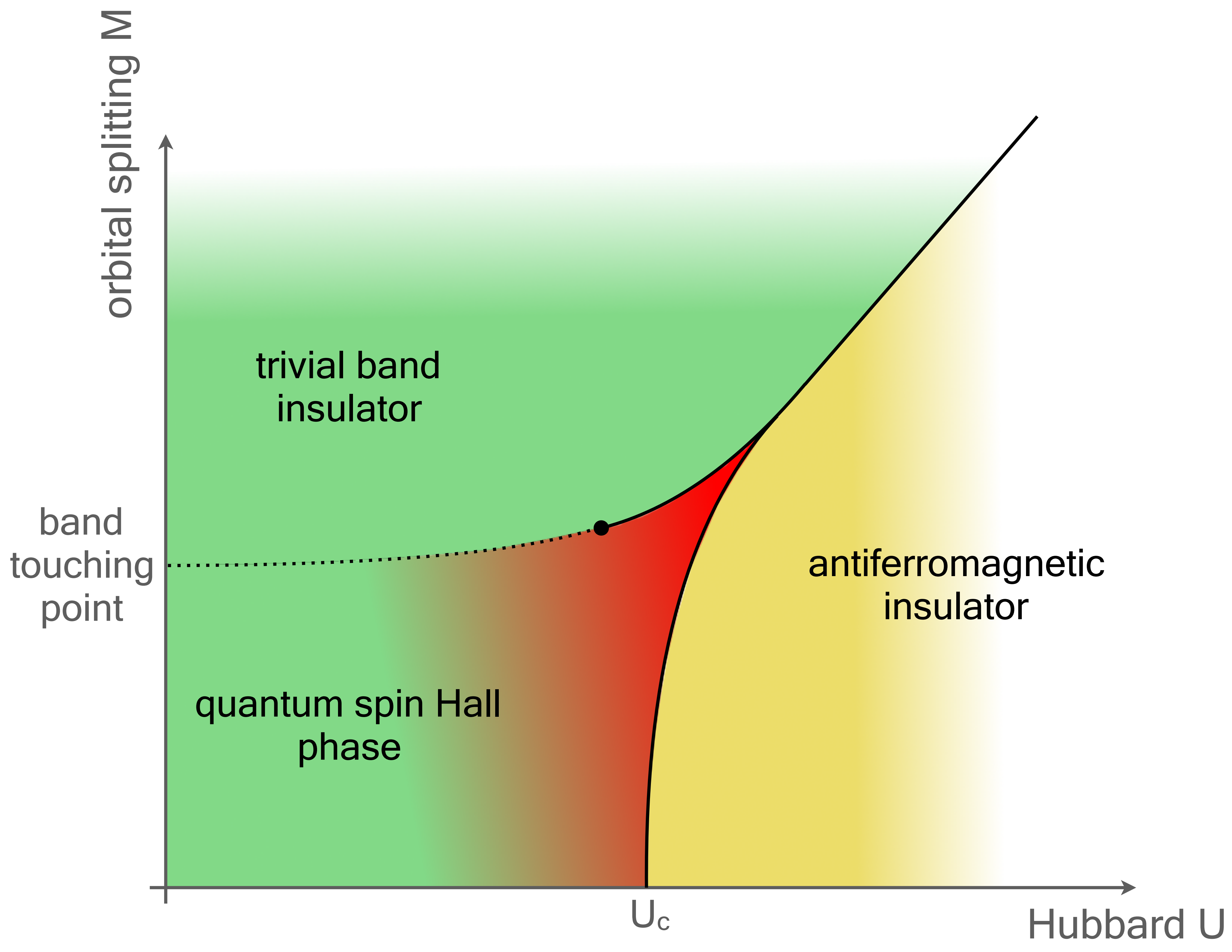


- QSHI and BI no longer smoothly connected
- Gap inversion occurring via a jump

1st-order QSH transition also in Xue&MacDonald PRL (2018)

Consequences on the topological phase transition

- gap closing: for $U<U_c$ smooth topological phase transition (green → green)
- no semimetal for $U>U_c$ when the $\mathbb{Z}_2$ topological invariant changes (green → red)!
- new termodynamics, beyond single-particle effective description



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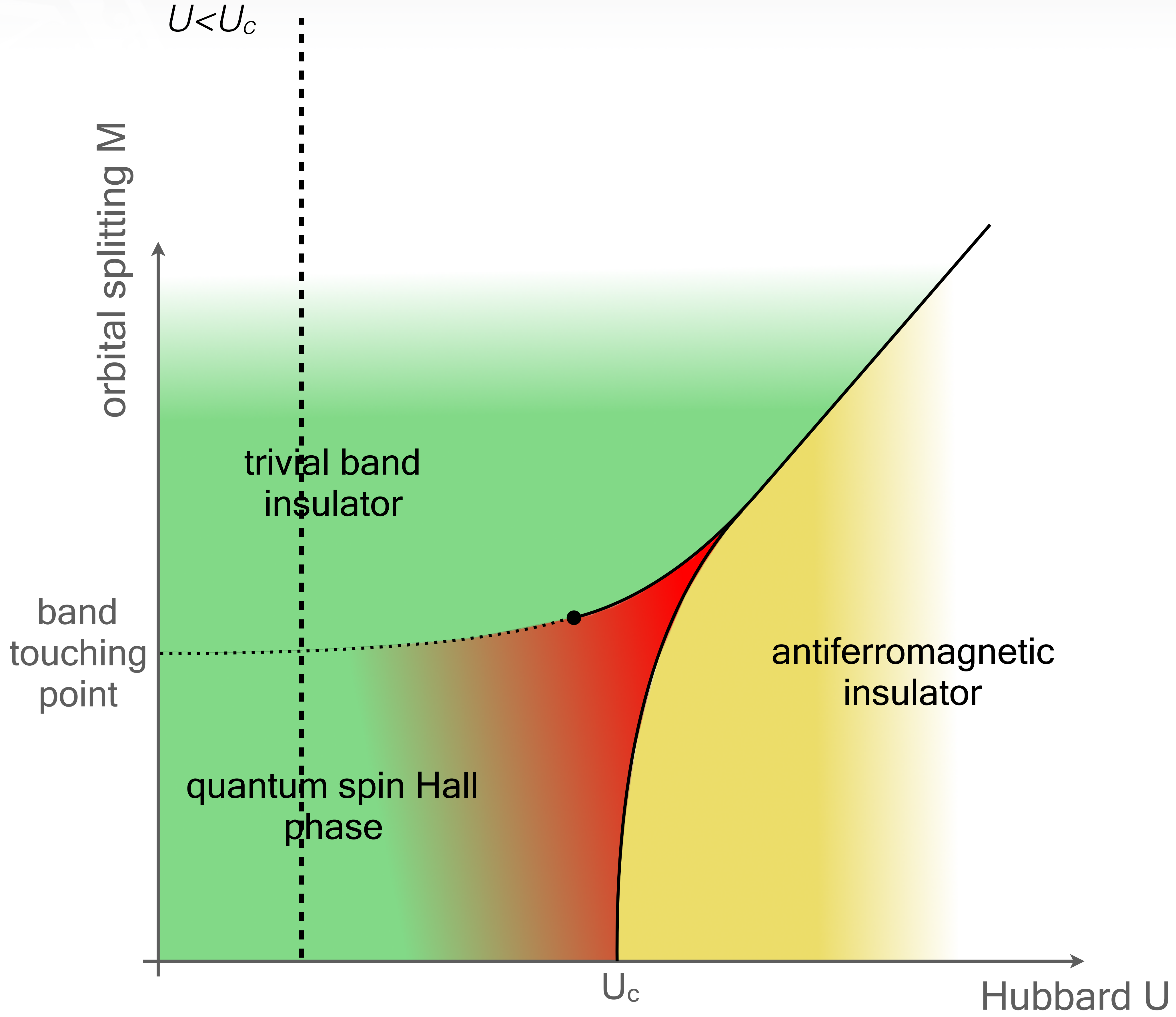

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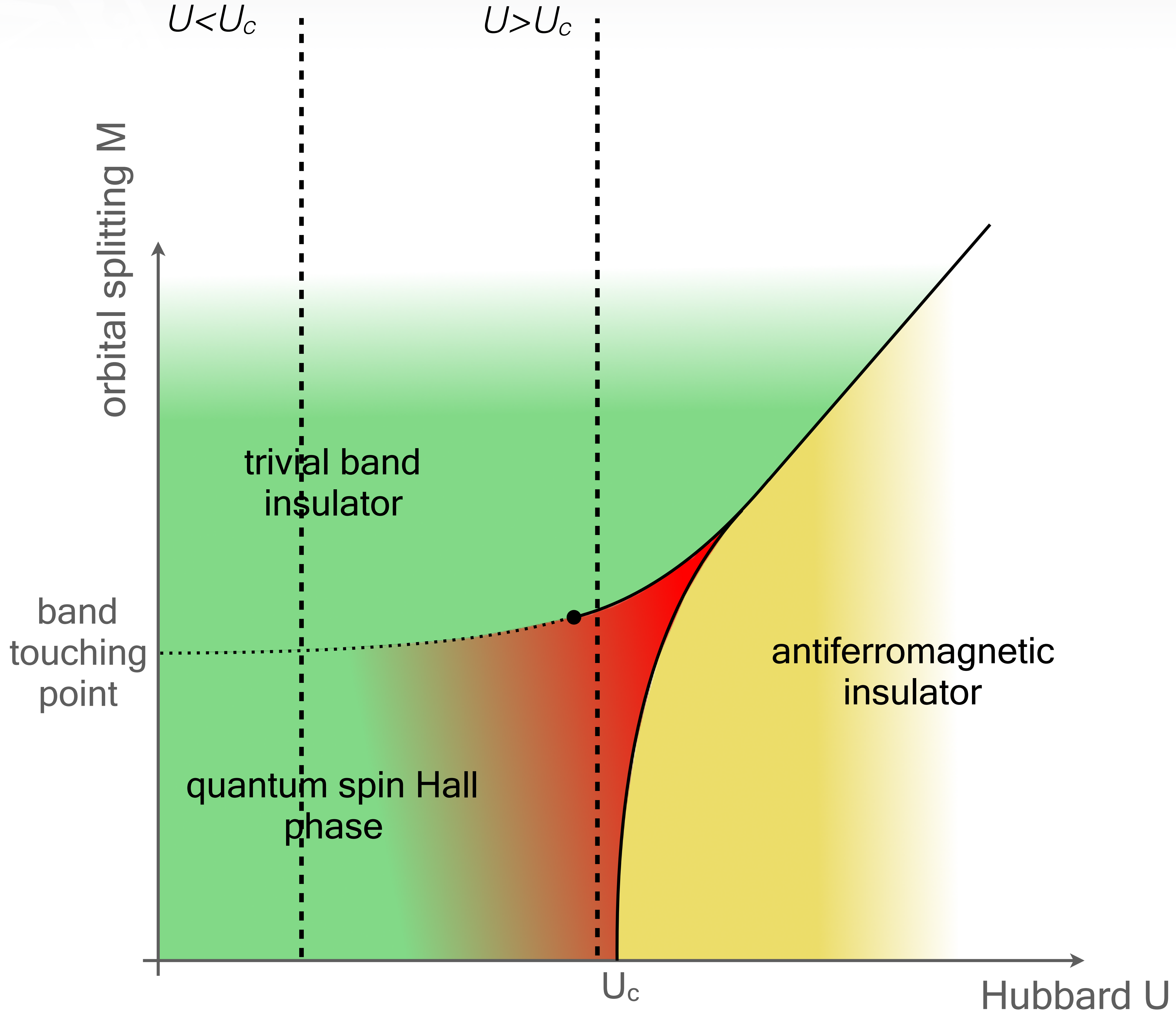

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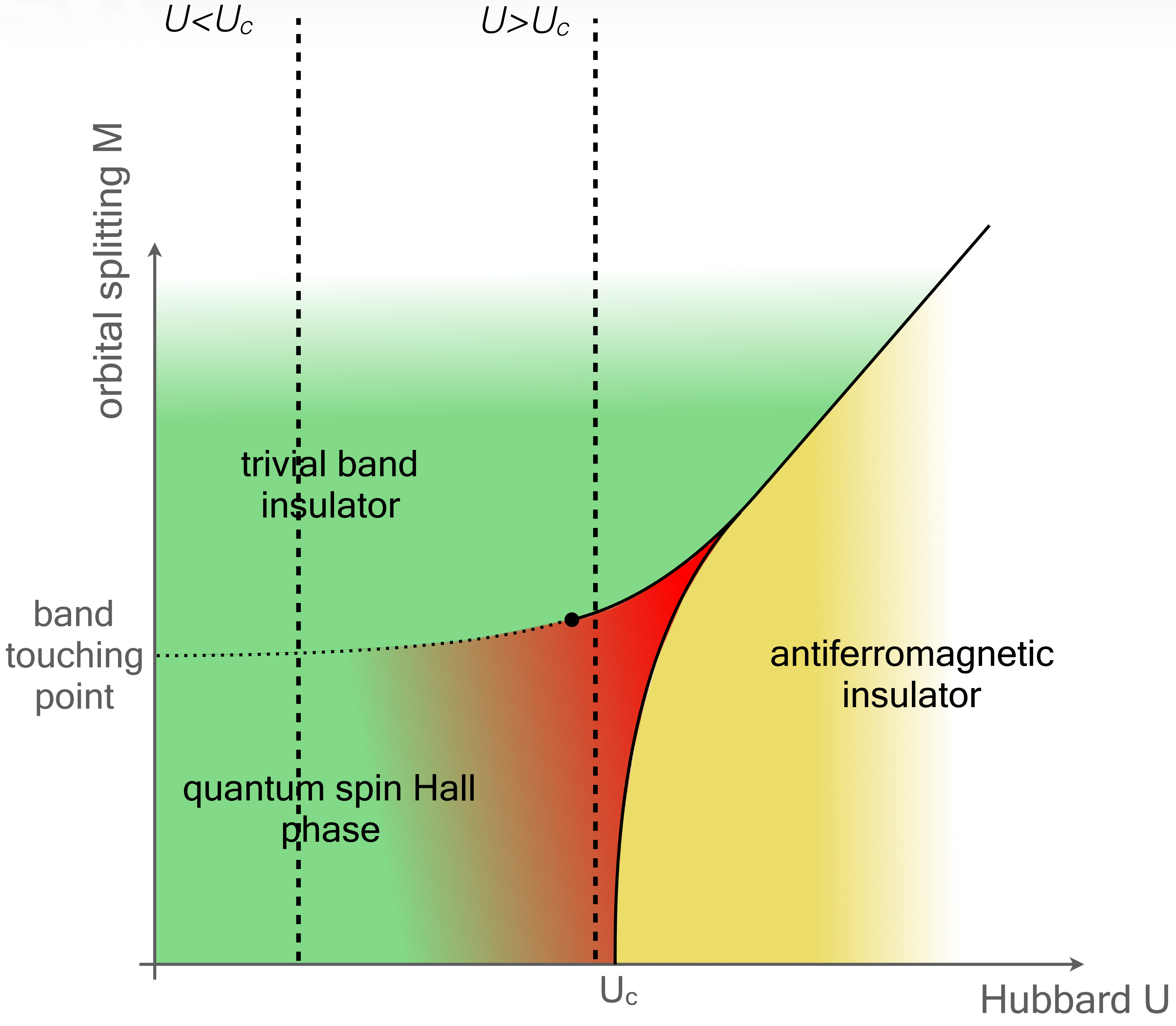

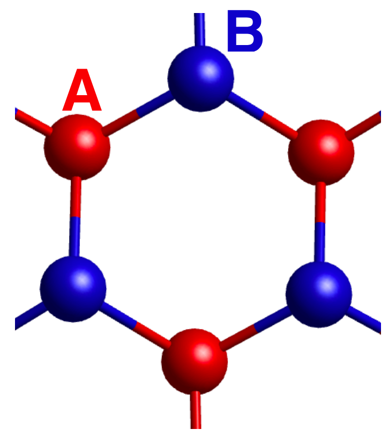

$$H = t \sum_{\langle ij \rangle,\alpha} c^{\dagger}_{i,\alpha} c_{j,\alpha} + i\lambda_{\mathrm{SO}} \sum_{\langle\langle ij \rangle\rangle,\alpha\alpha'} \nu_{ij} c^{\dagger}_{i,\alpha} s^{z}_{\alpha\alpha'} c_{j,\alpha'} + i\lambda_R \sum_{\langle ij \rangle,\alpha\alpha'} c^{\dagger}_{i,\alpha} (\mathbf{s} \times \hat{\mathbf{d}}_{ij})^{z}_{\alpha\alpha'} c_{j,\alpha'}$$

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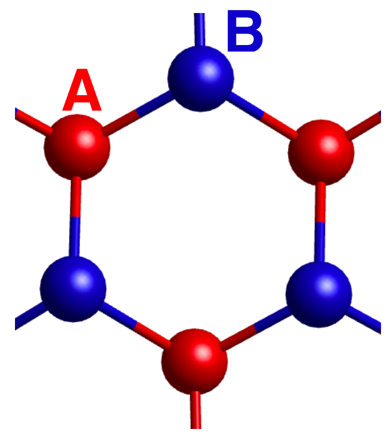
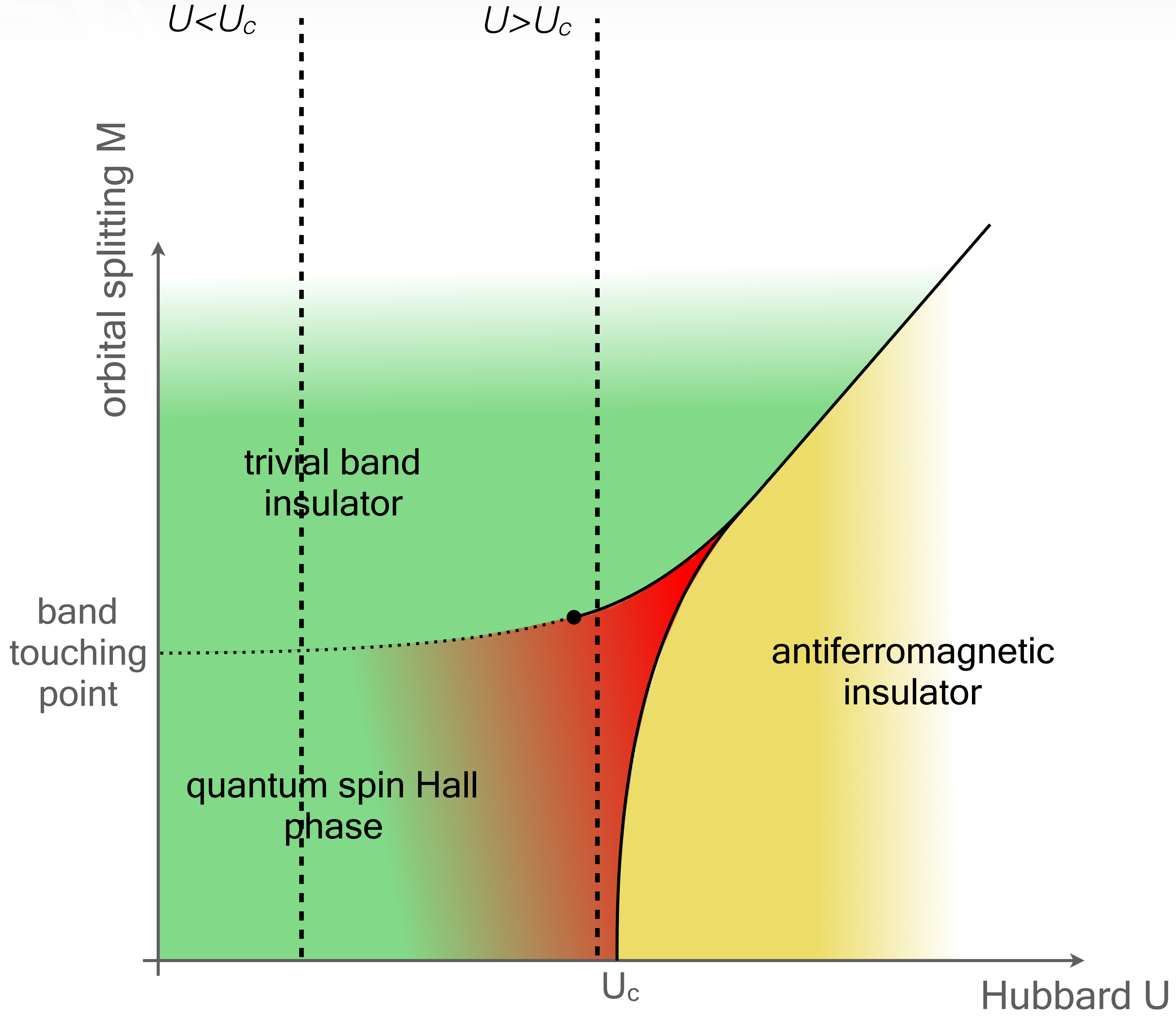
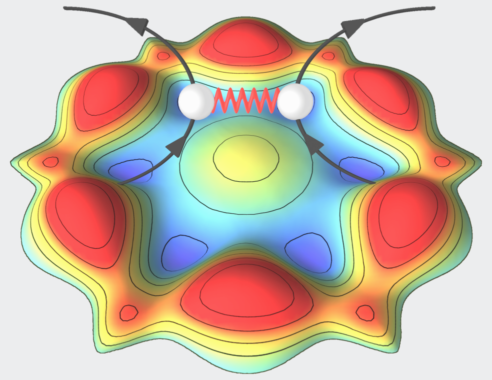




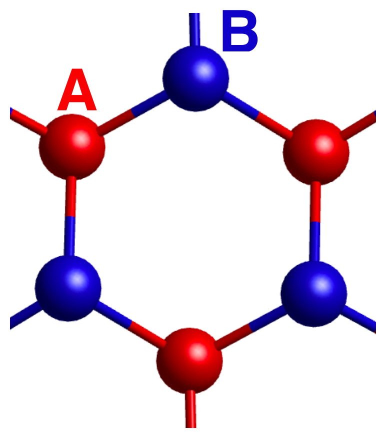
A/**B** splitting

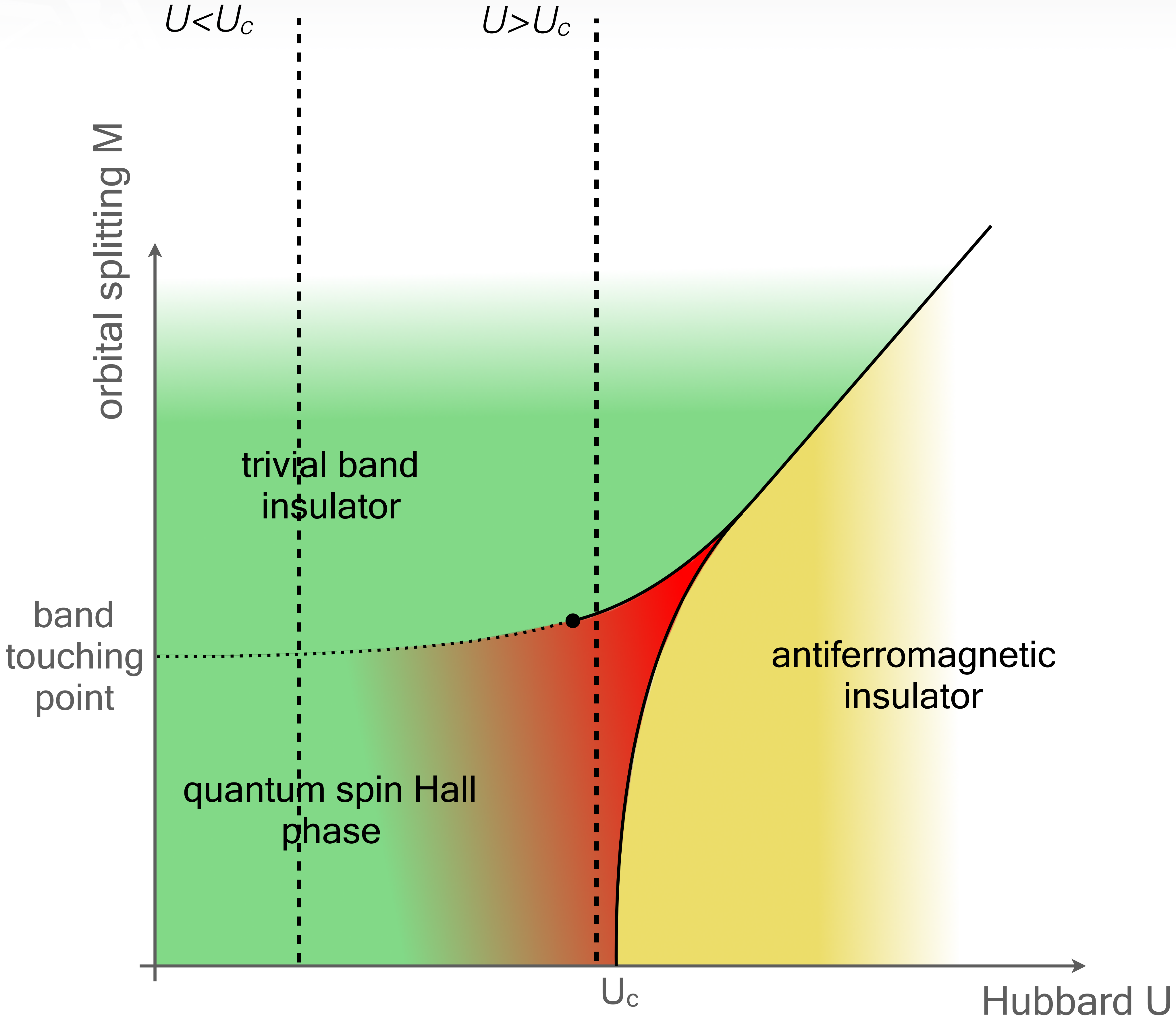
$$H = t\sum_{\langle ij\rangle,\alpha} c^\dagger_{i,\alpha}c_{j,\alpha} + i\lambda_{\mathrm{SO}}\sum_{\langle\langle ij\rangle\rangle,\alpha\alpha'} \nu_{ij}c^\dagger_{i,\alpha}s^z_{\alpha\alpha'}c_{j,\alpha'} + i\lambda_R\sum_{\langle ij\rangle,\alpha\alpha'} c^\dagger_{i,\alpha}(\mathbf{s}\times\hat{\mathbf{d}}_{ij})^z_{\alpha\alpha'}c_{j,\alpha'} + \mathrm{M}\sum_{i,\alpha}^{\mathbf{A},\,\mathbf{B}}\xi_i c^\dagger_{i,\alpha}c_{i,\alpha}$$

Consequences on the topological phase transition

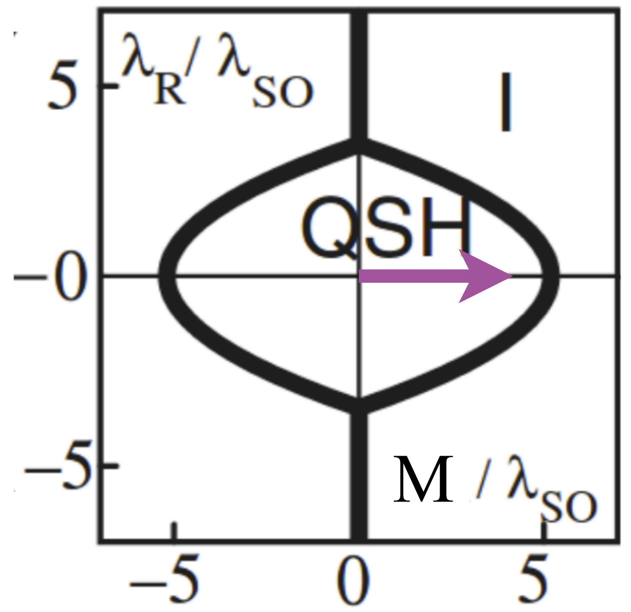


- gap closing: for $U<U_c$ smooth topological phase transition (green → green)
- no semimetal for $U>U_c$ when the $\mathbb{Z}_2$ topological invariant changes (green → red)!
- new termodynamics, beyond single-particle effective description
- analogy with the Kane-Mele-Hubbard and Haldane-Hubbard models





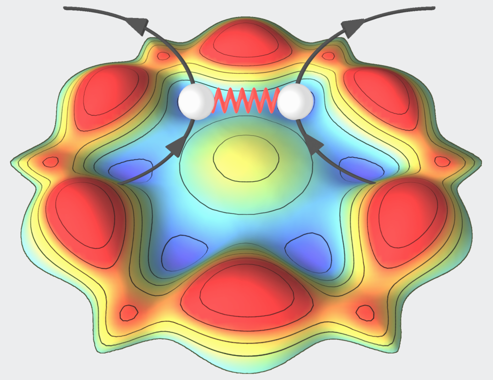
A/B splitting



C. Kane & E. Mele, PRL (2005)

$$H = t \sum_{\langle ij\rangle,\alpha} c^\dagger_{i,\alpha} c_{j,\alpha} + i\lambda_{SO} \sum_{\langle\langle ij\rangle\rangle,\alpha\alpha'} \nu_{ij} c^\dagger_{i,\alpha} s^z_{\alpha\alpha'} c_{j,\alpha'} + i\lambda_R \sum_{\langle ij\rangle,\alpha\alpha'} c^\dagger_{i,\alpha} (\mathbf{s}\times\hat{\mathbf{d}}_{ij})^z_{\alpha\alpha'} c_{j,\alpha'} + \mathrm{M} \overset{\text{A, B}}{\sum_{i,\alpha}} \xi_i c^\dagger_{i,\alpha} c_{i,\alpha}$$

Consequences on the topological phase transition



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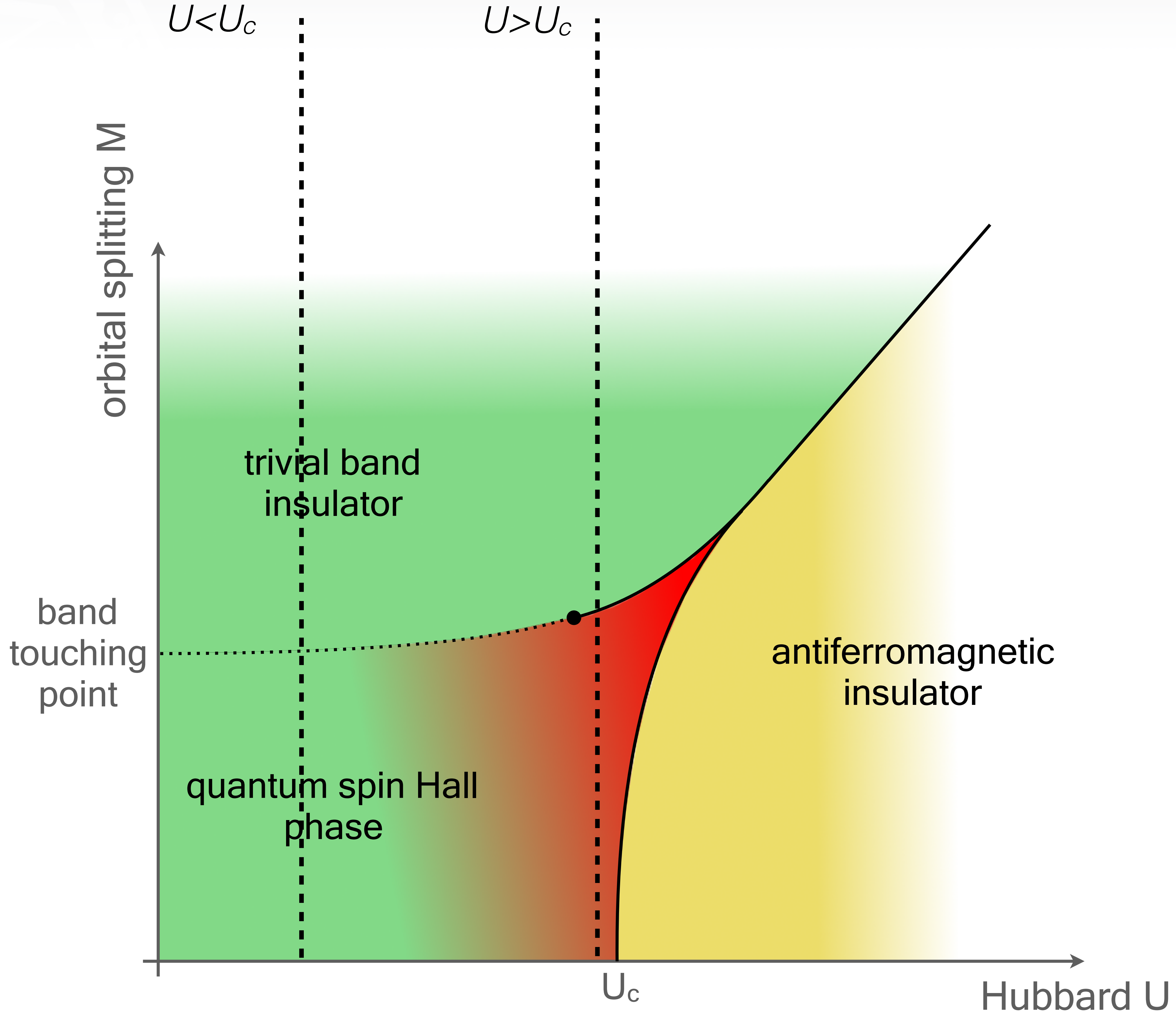
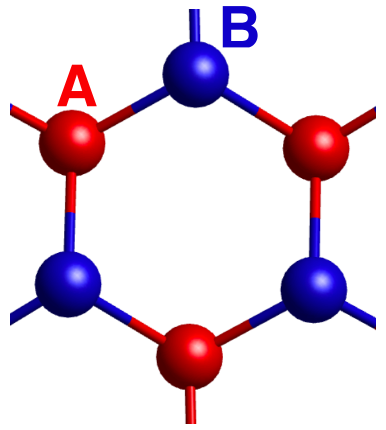
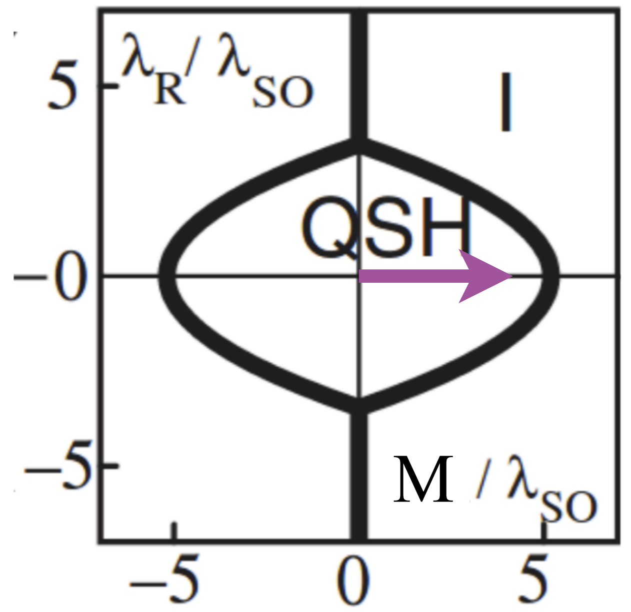


simpler “single-orbital” interaction term in this case:



$$U\sum_i n_{i,\uparrow}n_{i,\downarrow}$$

A/B splitting



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Consequences on the topological phase transition

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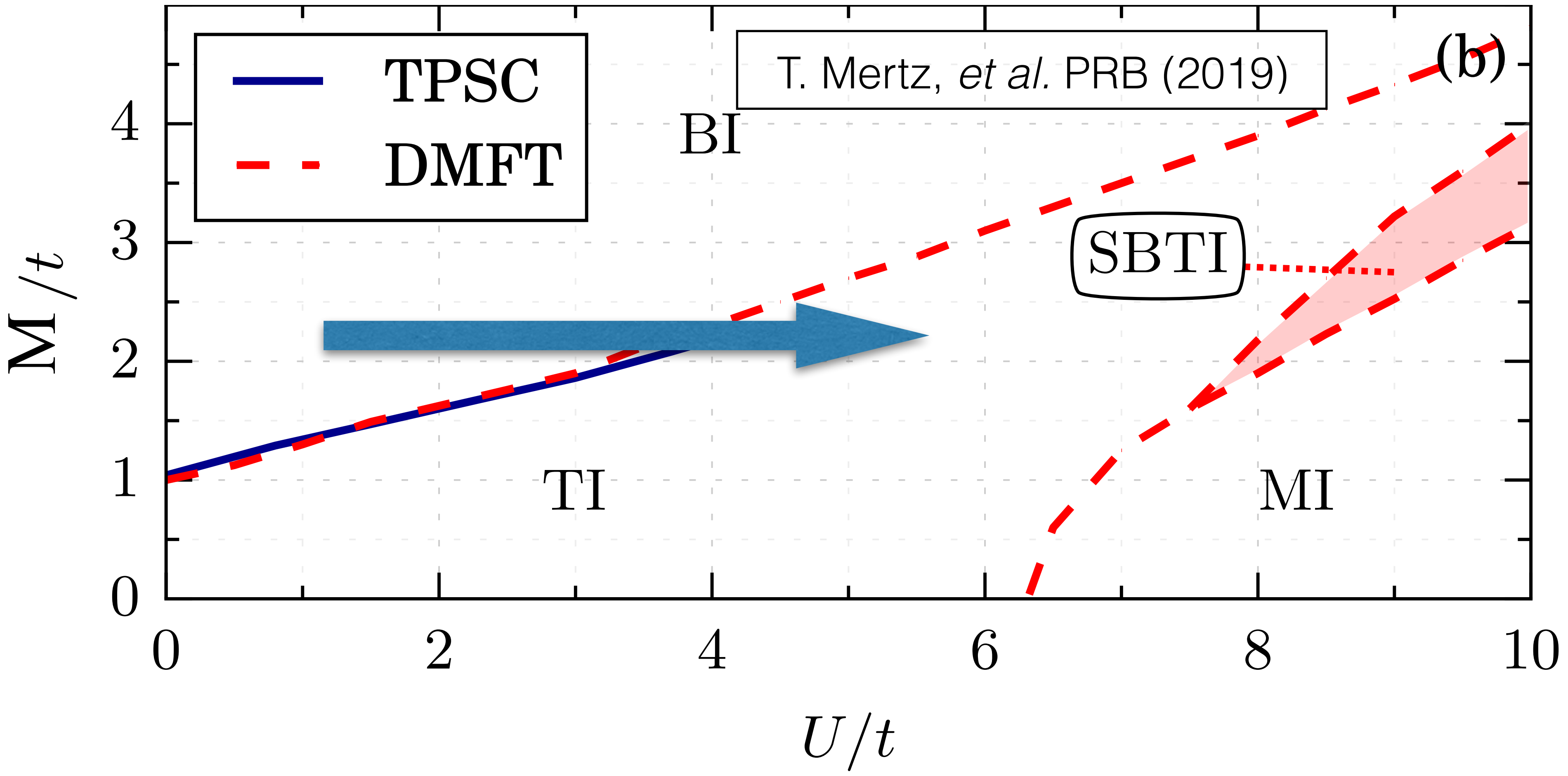
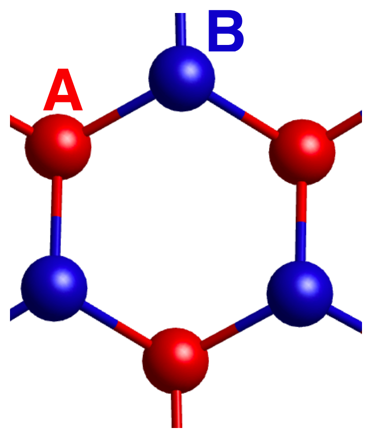


suppression of staggered potential and U-driven TI phase

simpler "single-orbital" interaction term in this case:



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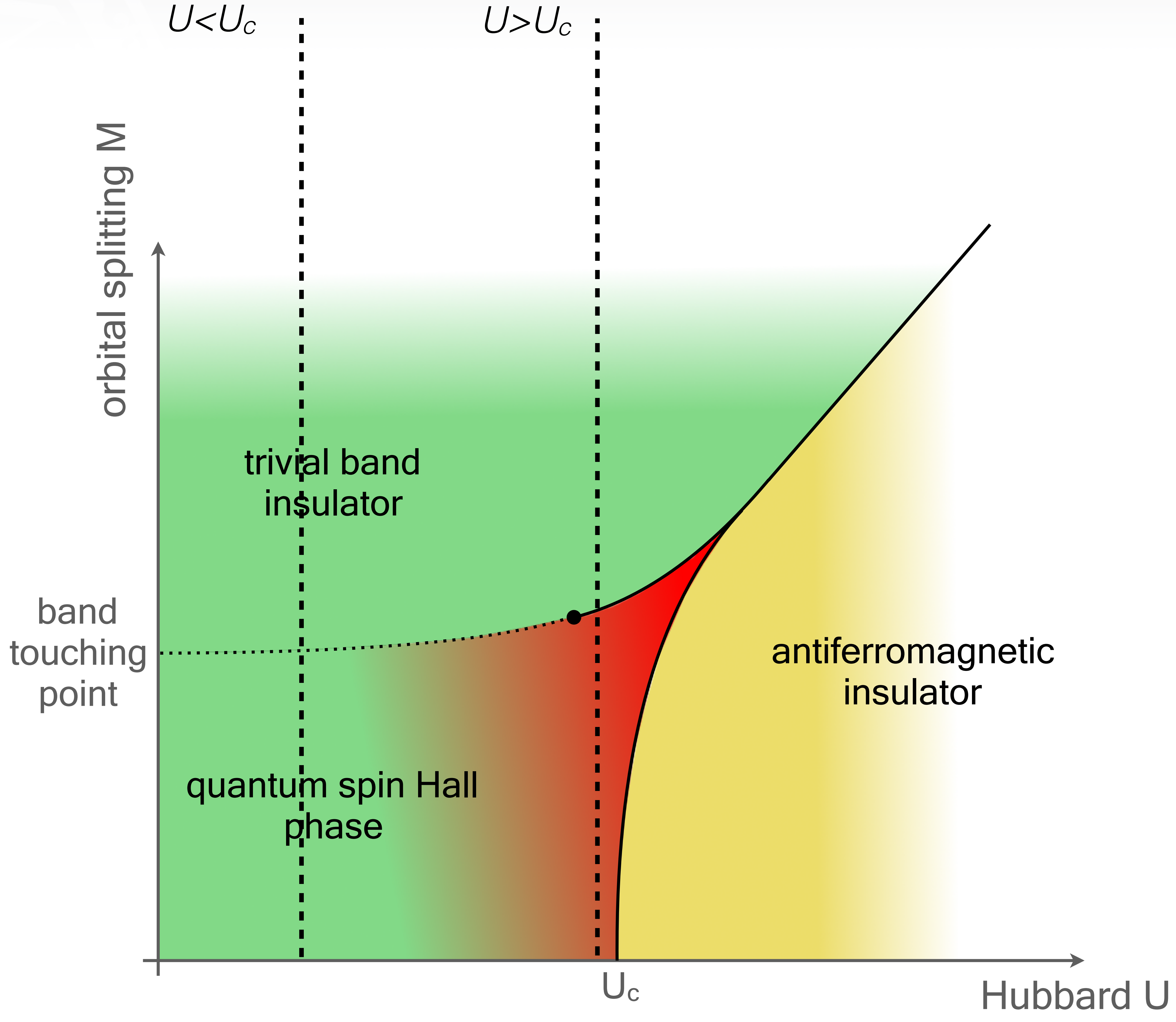

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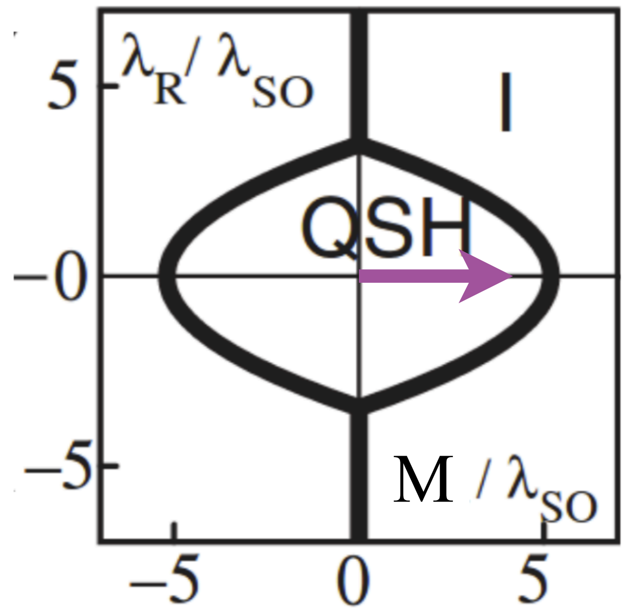

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Material realization?

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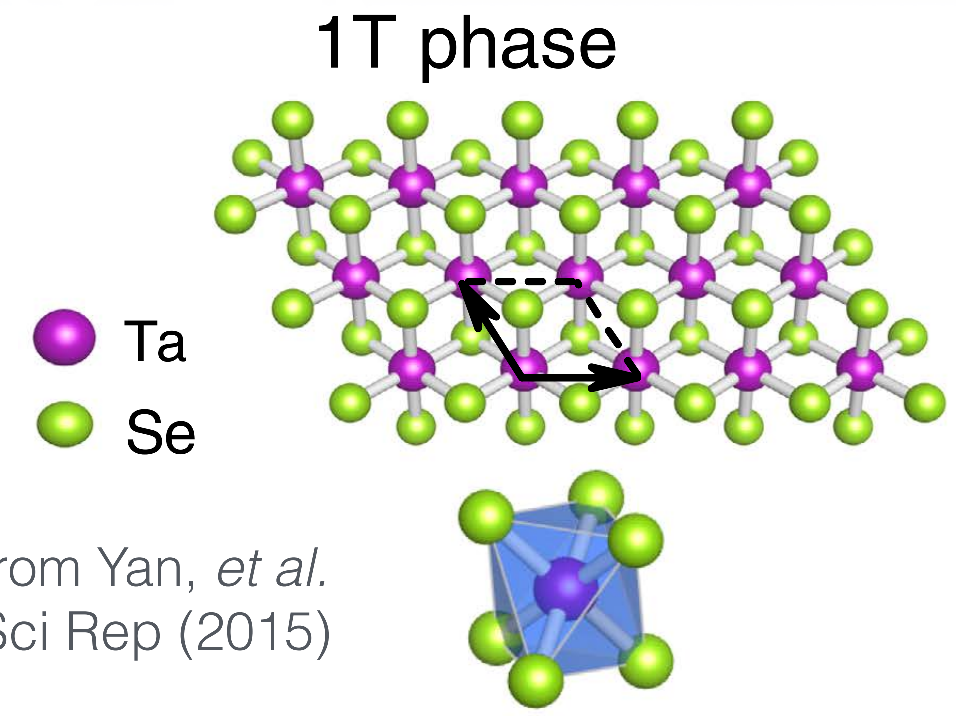
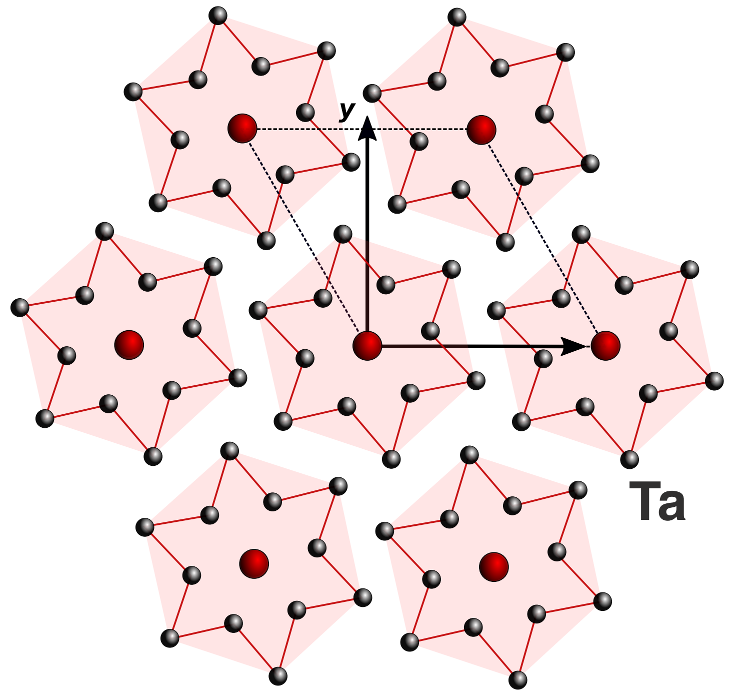


from Yan, *et al.*
Sci Rep (2015)



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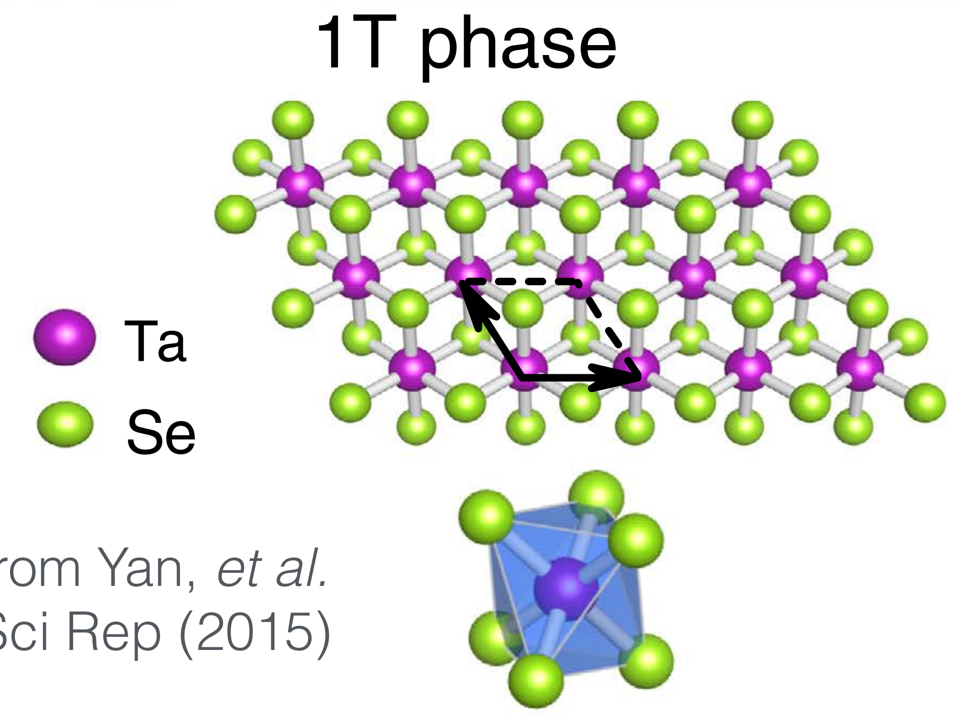

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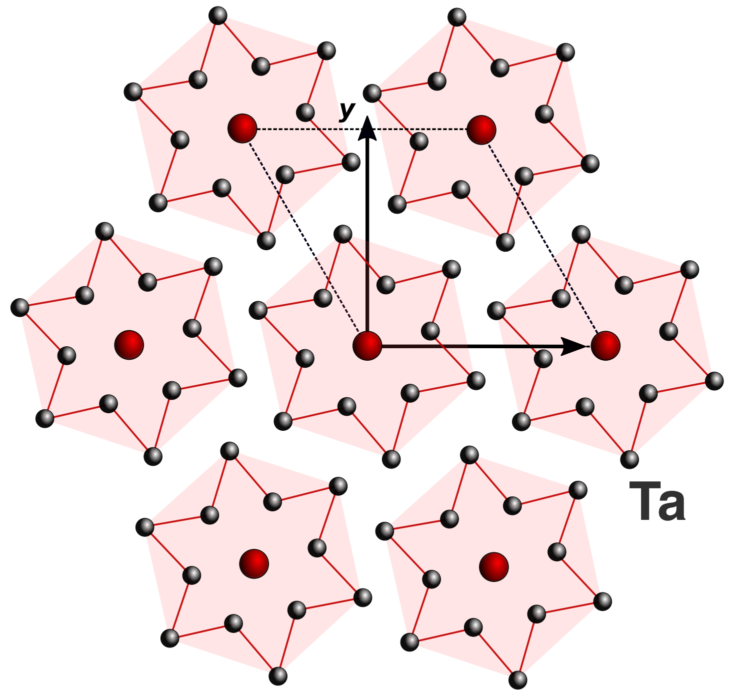

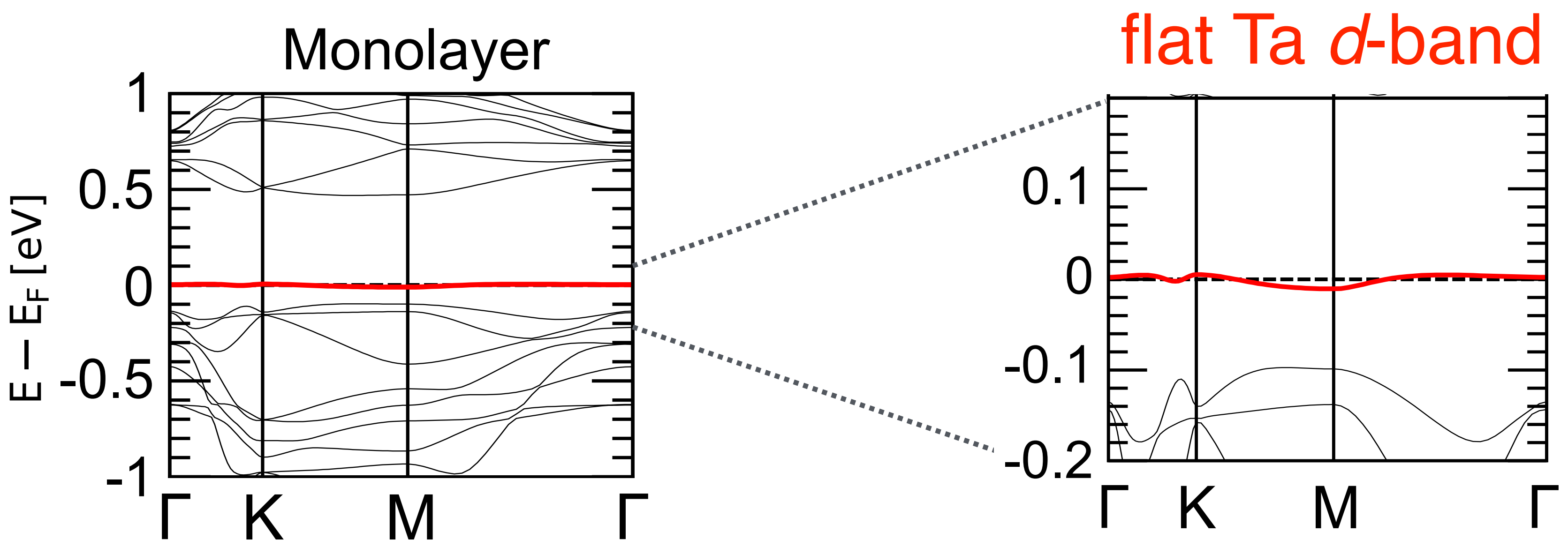

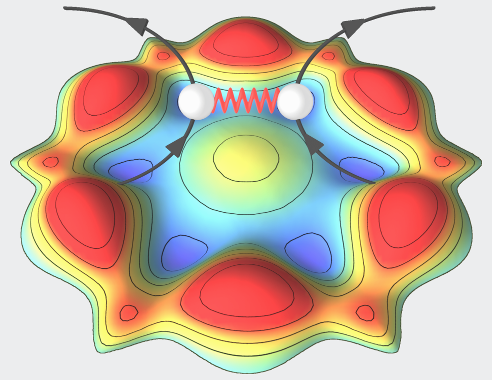

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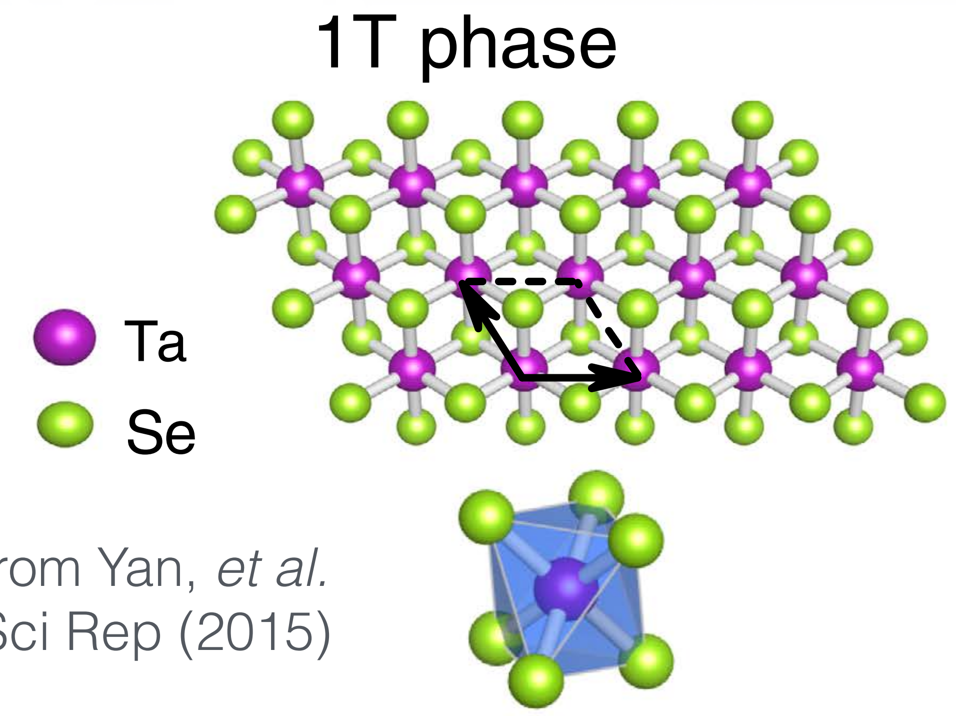

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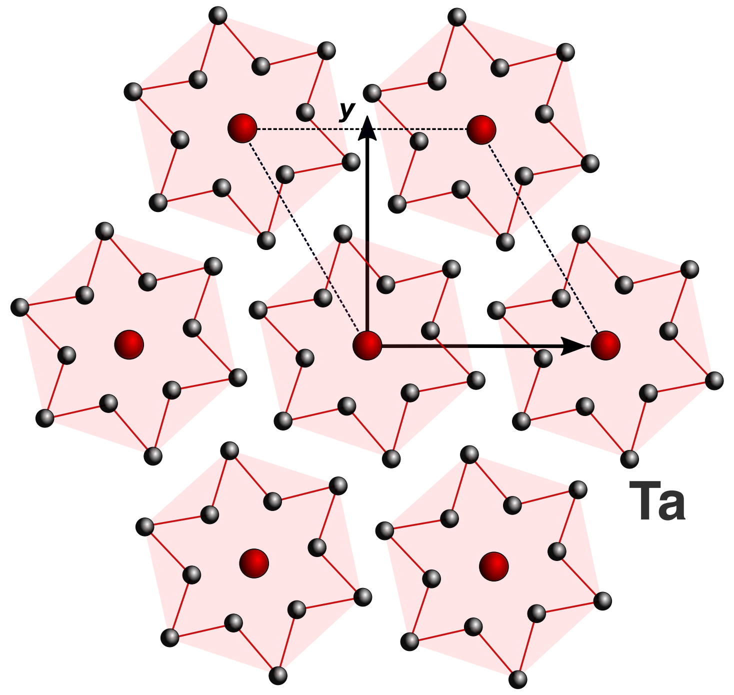

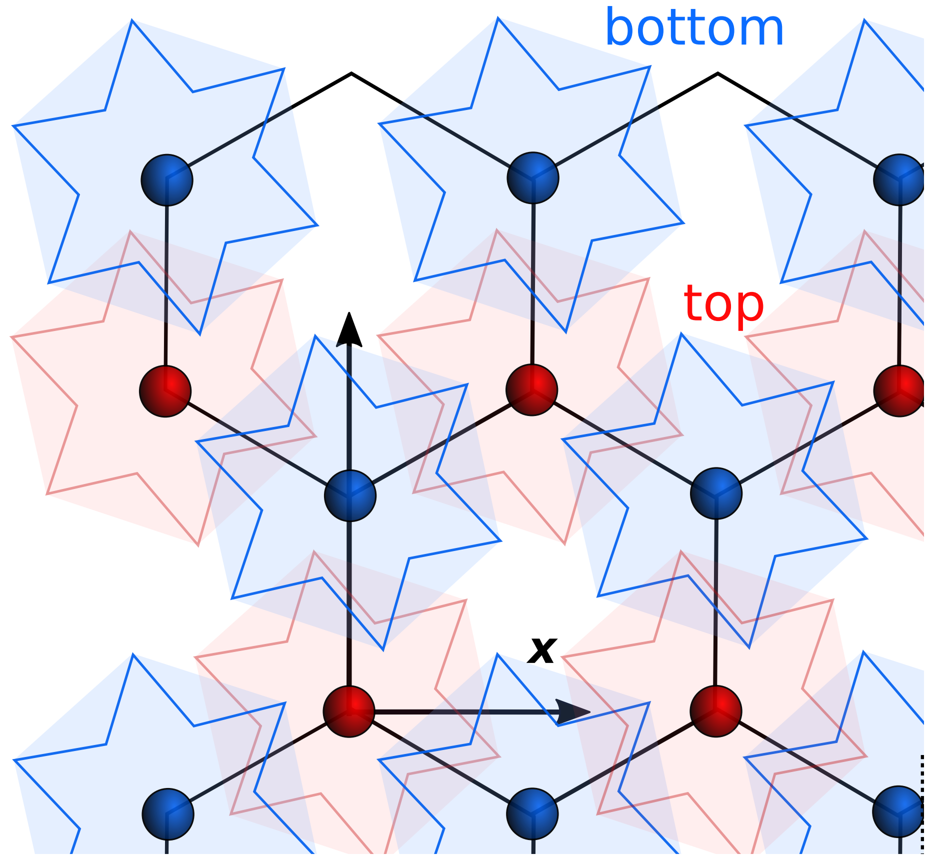

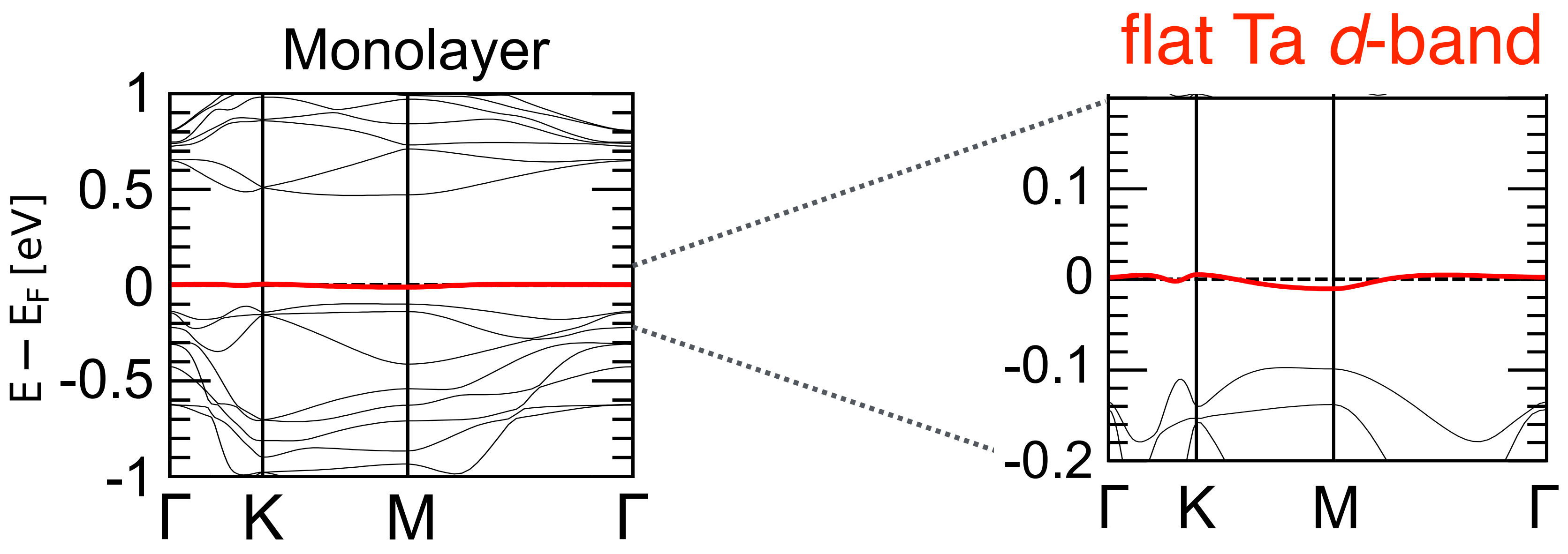

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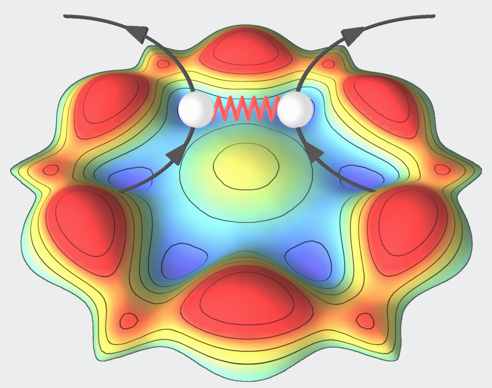

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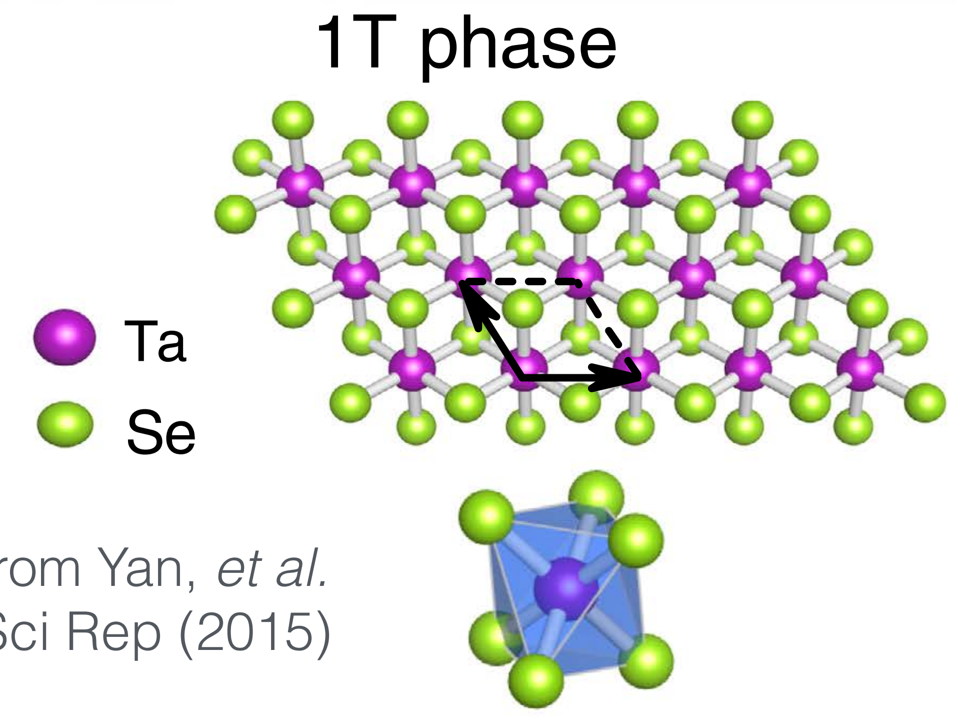

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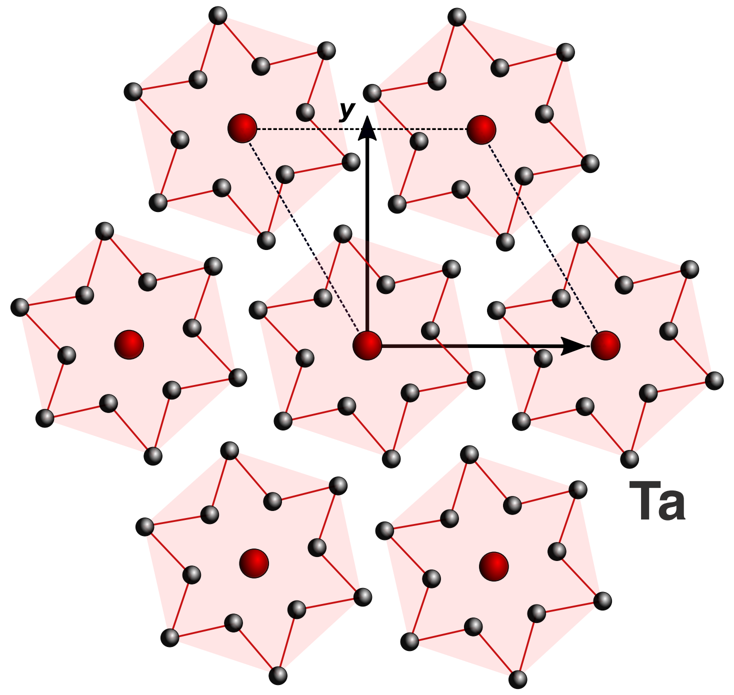
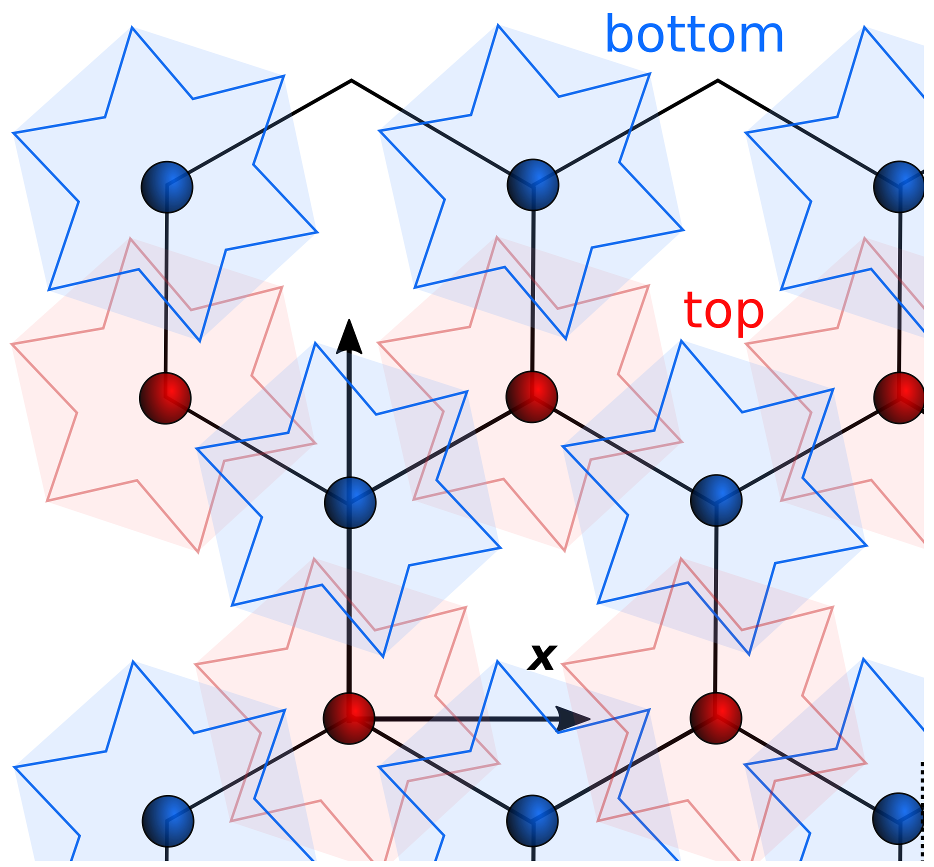
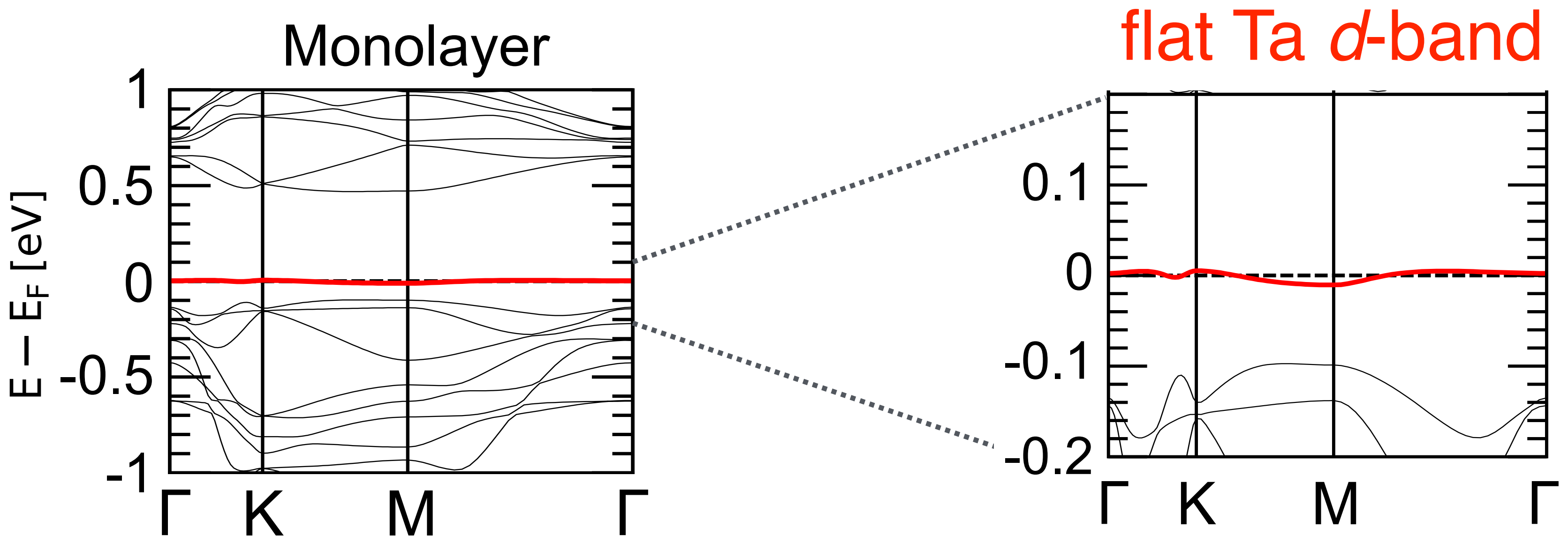
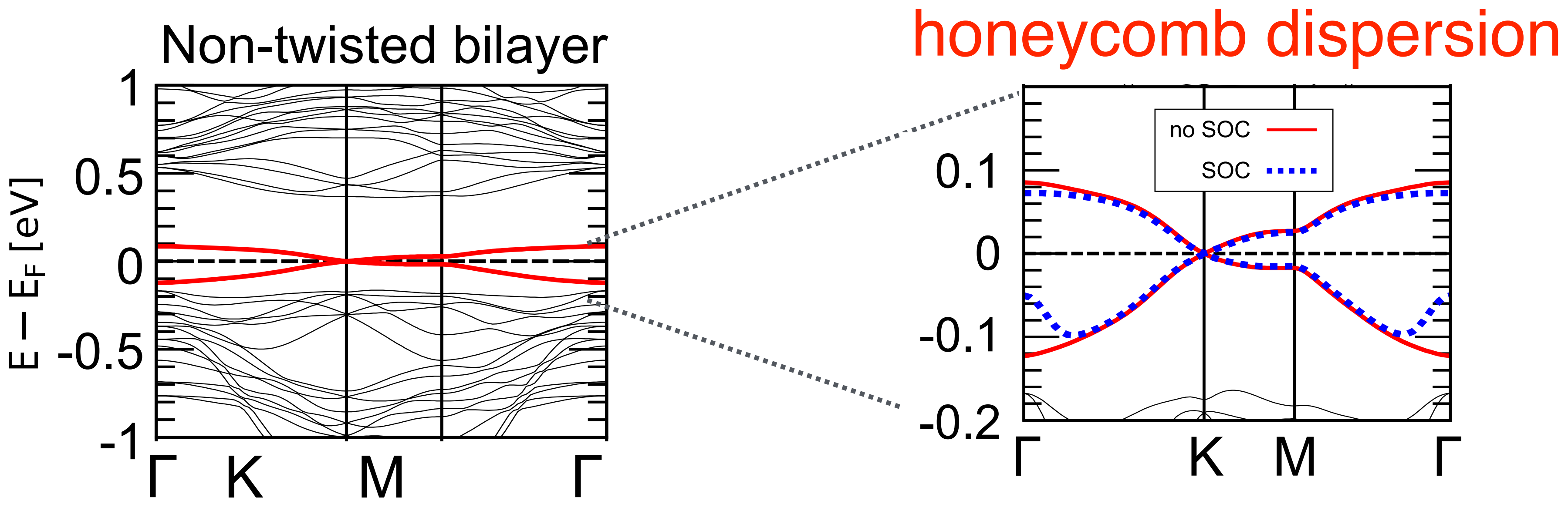




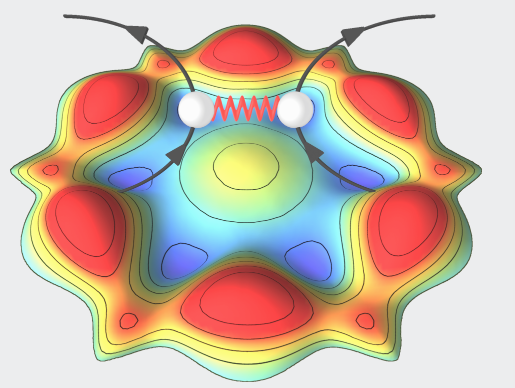
- “deconfinement” of Mott localized electrons into correlated Dirac fermions



opposite strategy w.r.t. twisted bilayer graphene



Material realization?



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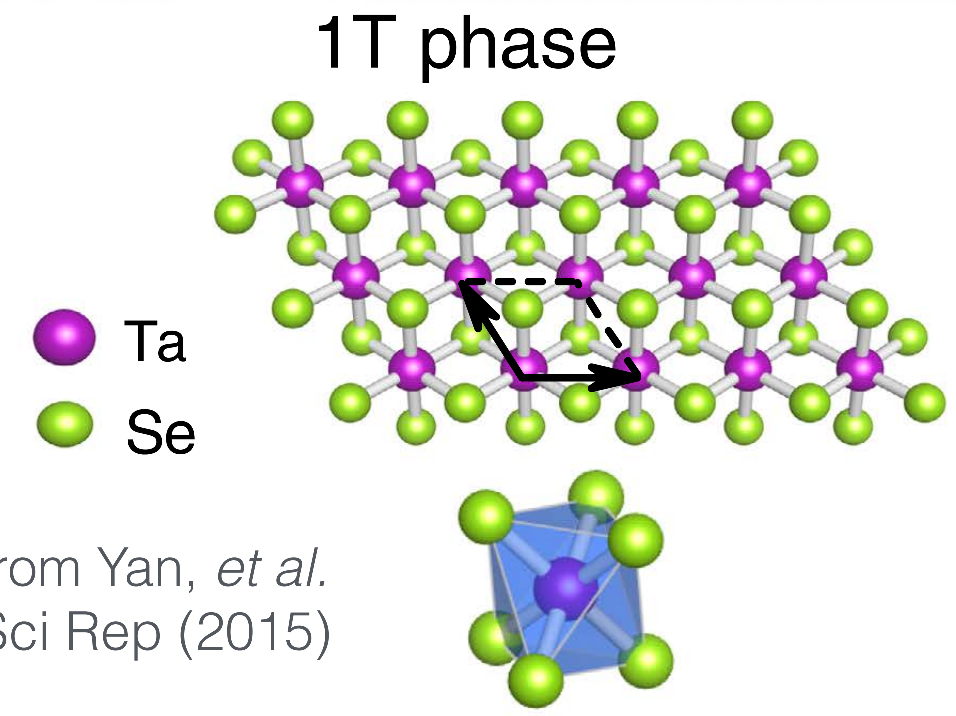

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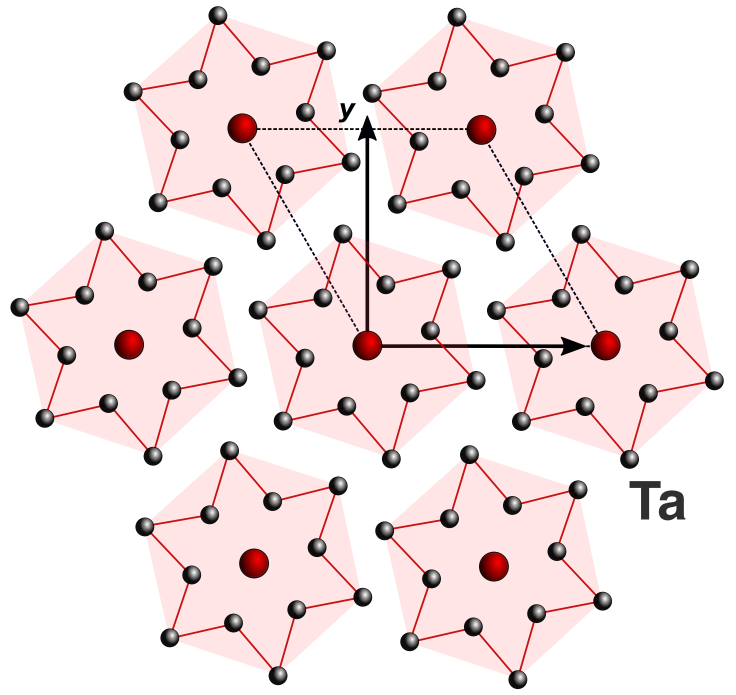
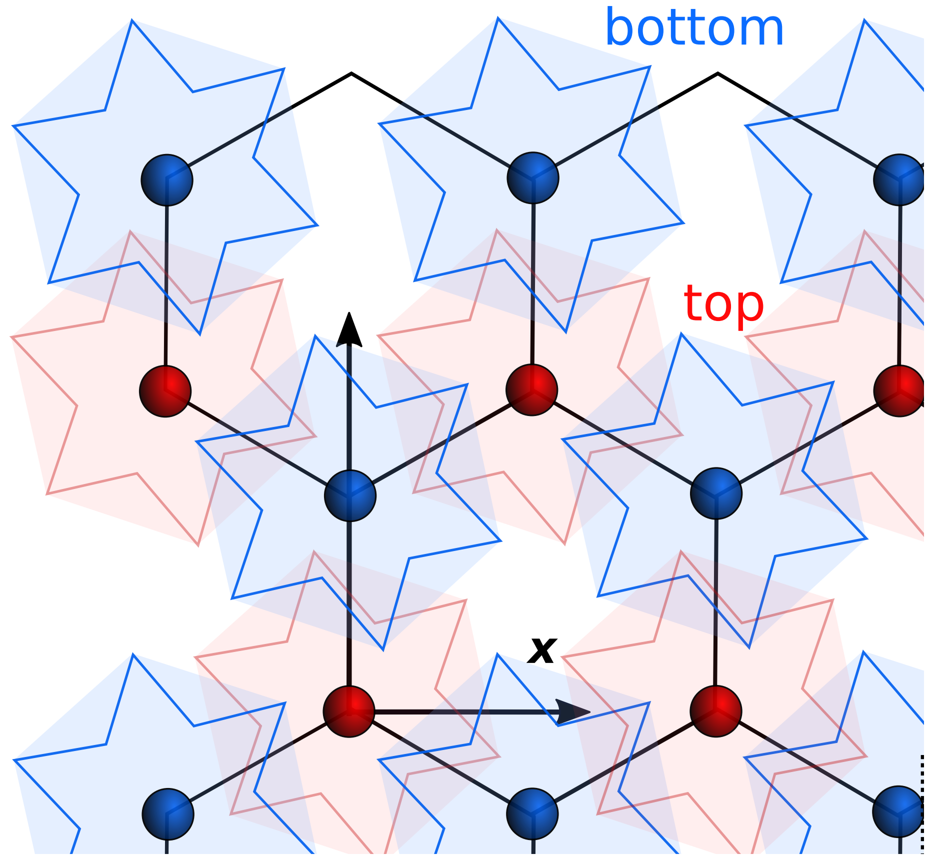
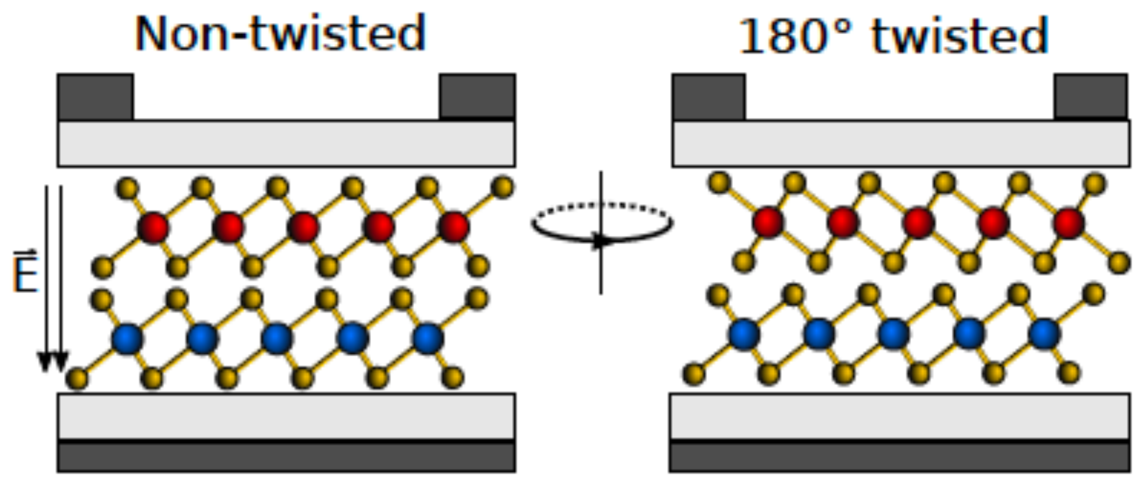
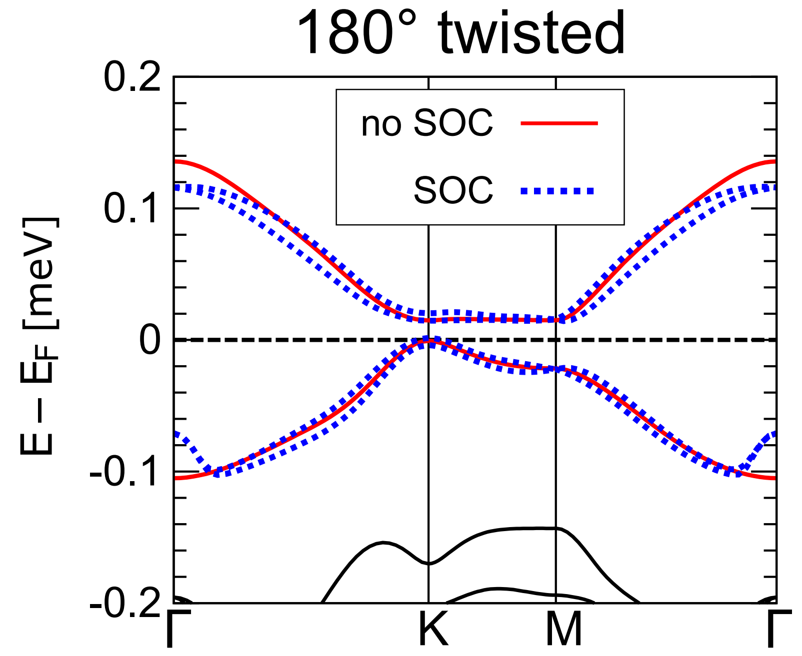






- twisting breaks inversion symmetry and opens a gap



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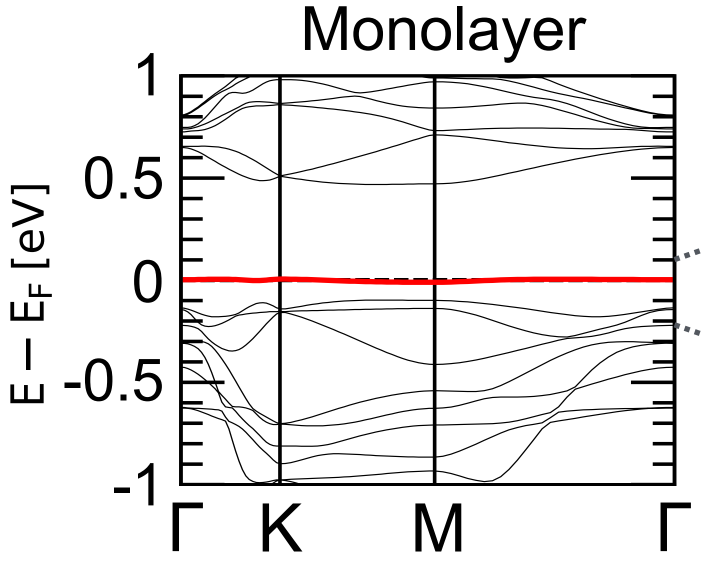

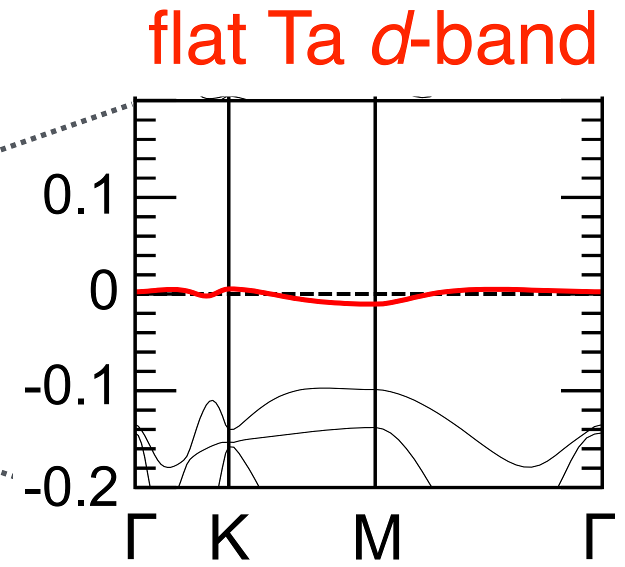

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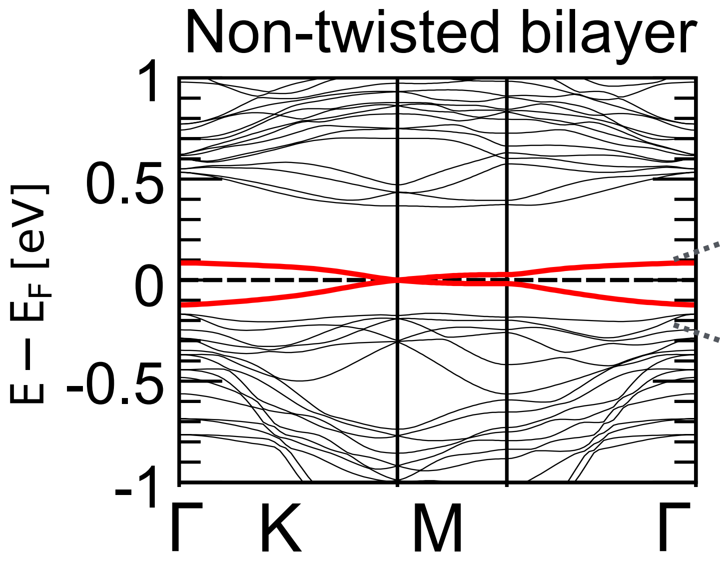
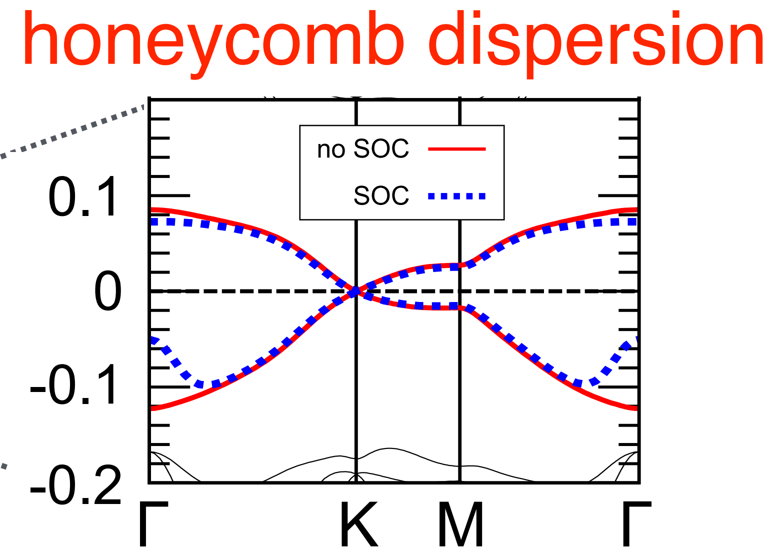
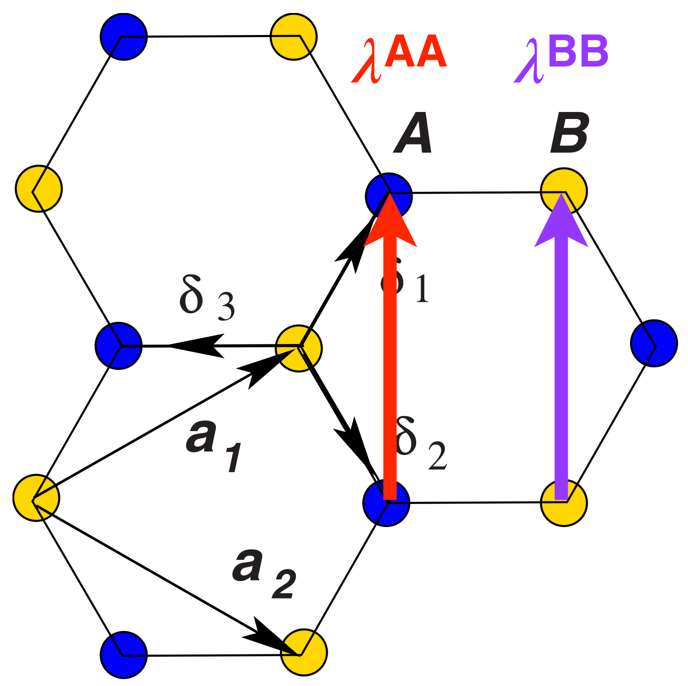
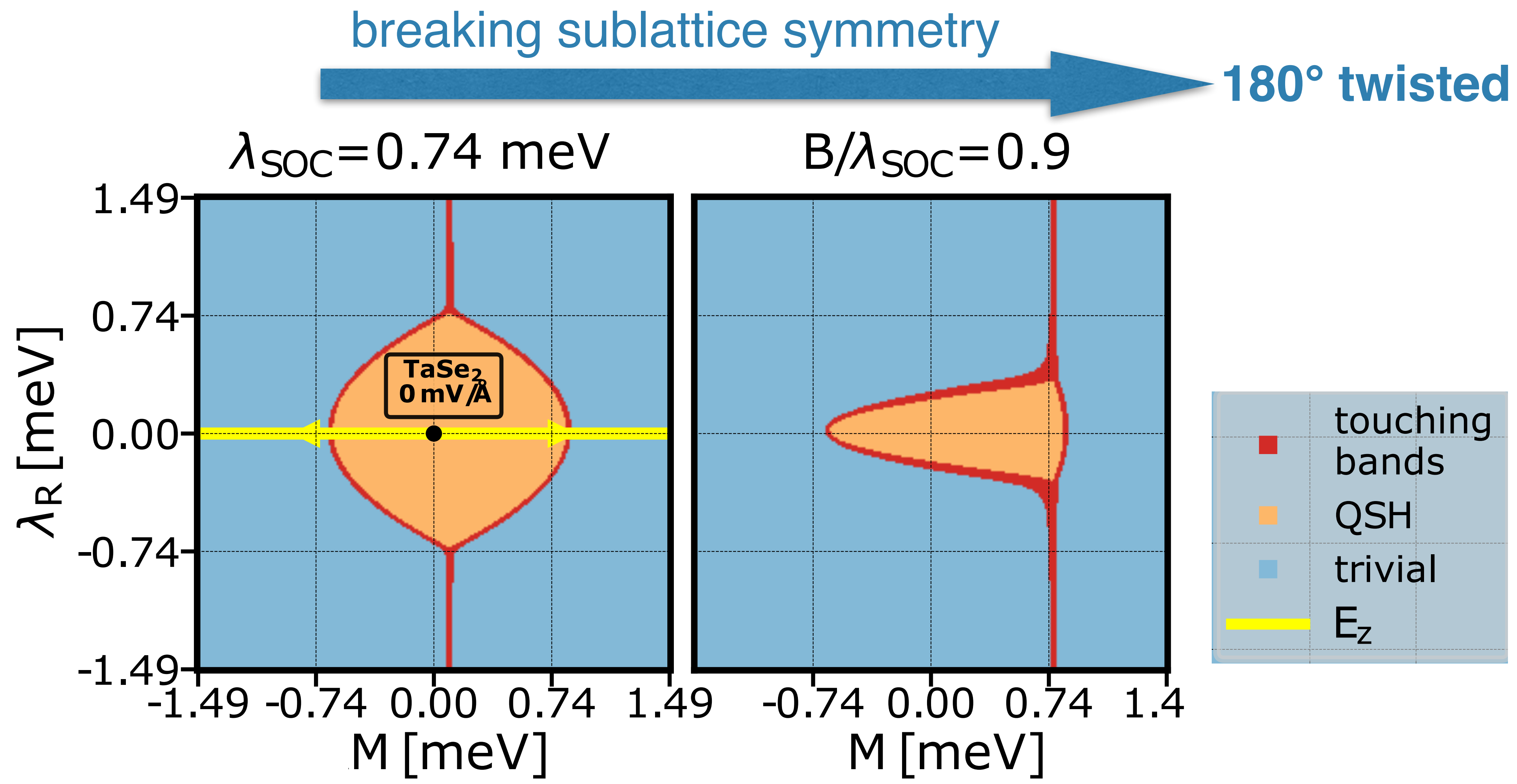




Material realization?

- we can tune M by means of electric field along *z* (~1-4 meV/Å)
- from D_{6h} to C_{3v}





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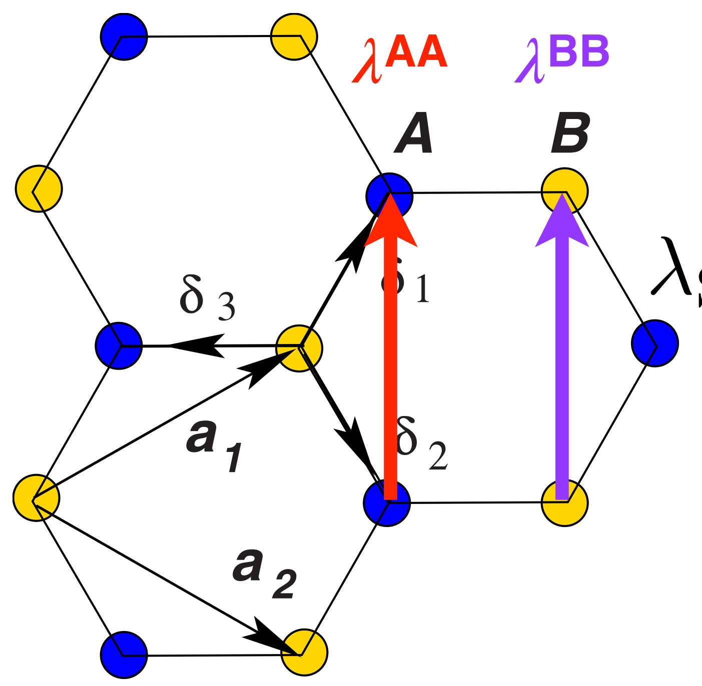
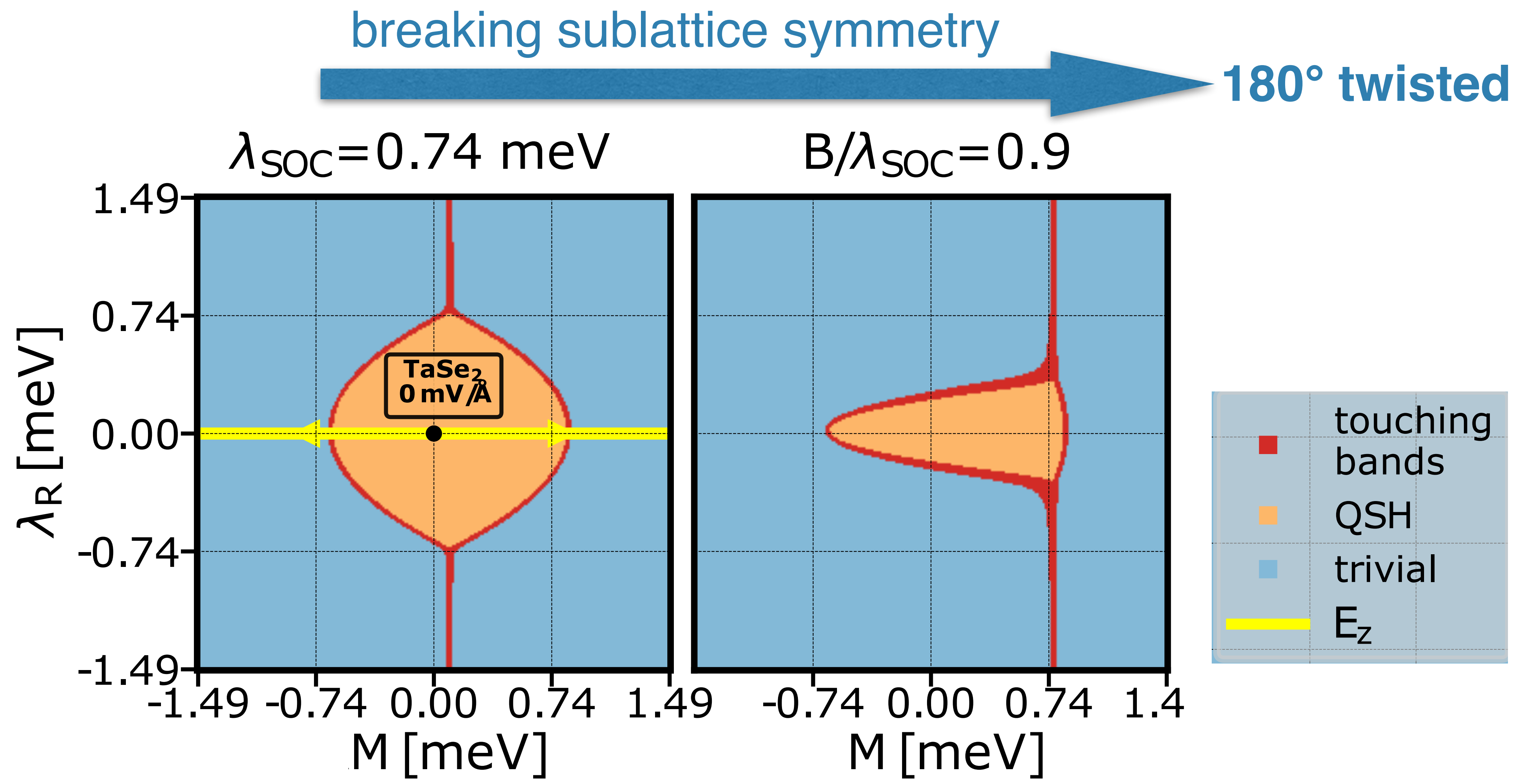


Kane-Mele SOC
$\lambda_{soc} = (\lambda^{AA} + \lambda^{BB})/2$

$$\lambda_{\mathrm{SOC}} \cdot \tau_z^{\mathrm{K,\,K'}} \cdot \sigma_z^{\mathrm{spin}} \cdot S_z^{\mathrm{sublatt}}$$



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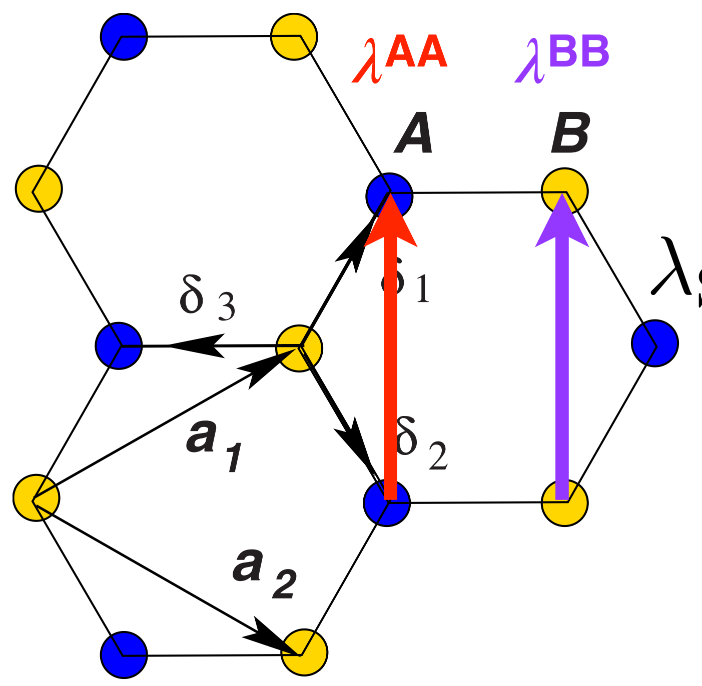

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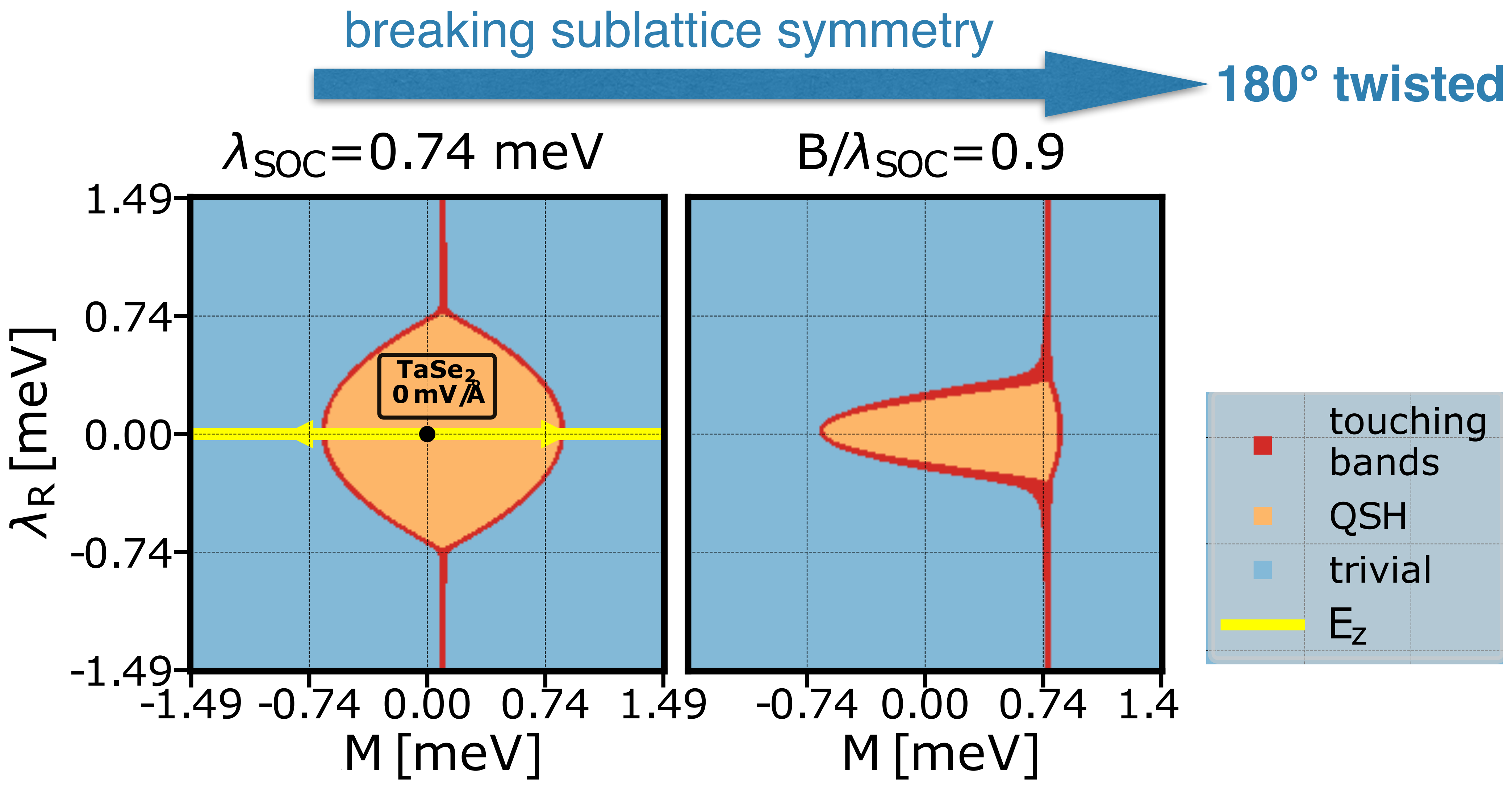
spin-valley term
$B = (\lambda^{AA}-\lambda^{BB})/2$



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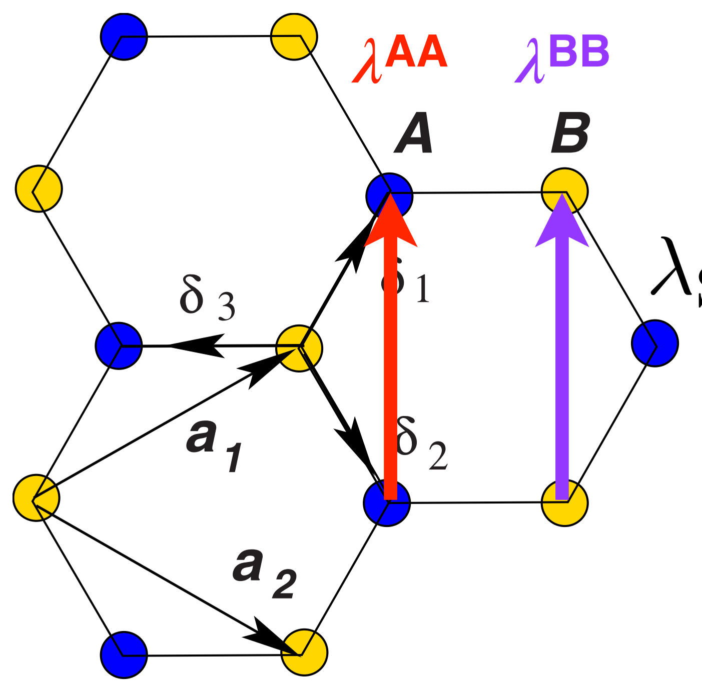

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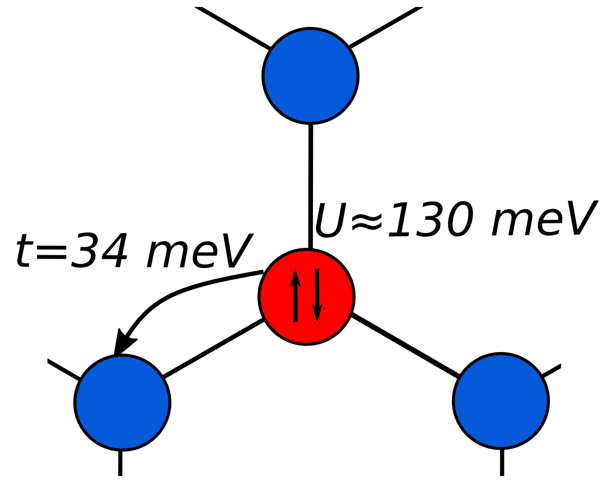
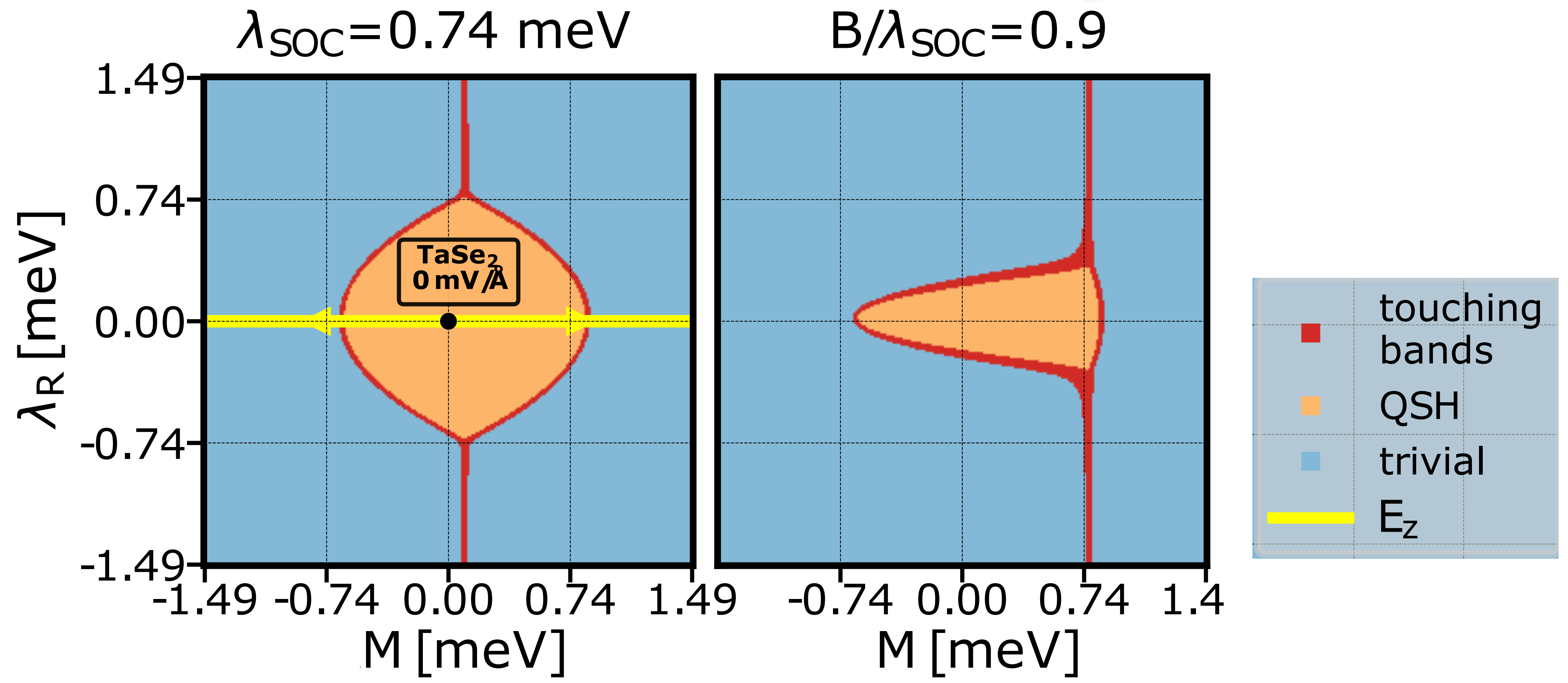
strong correlation



breaking sublattice symmetry → 180° twisted



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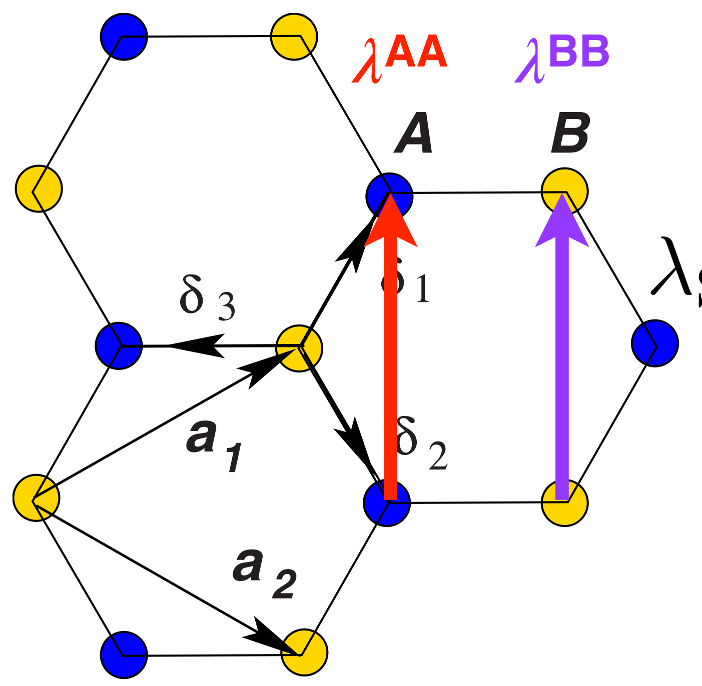

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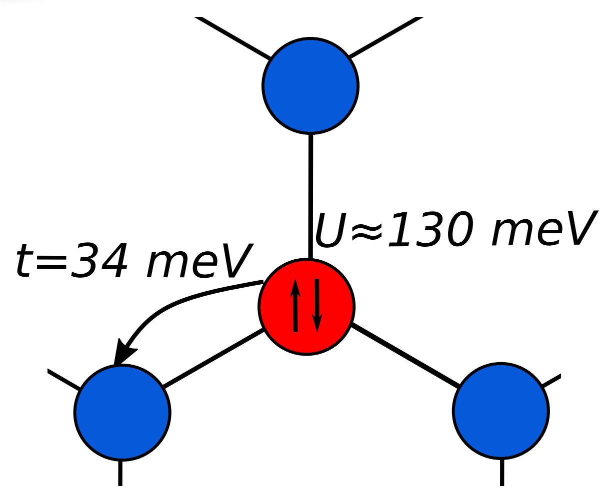

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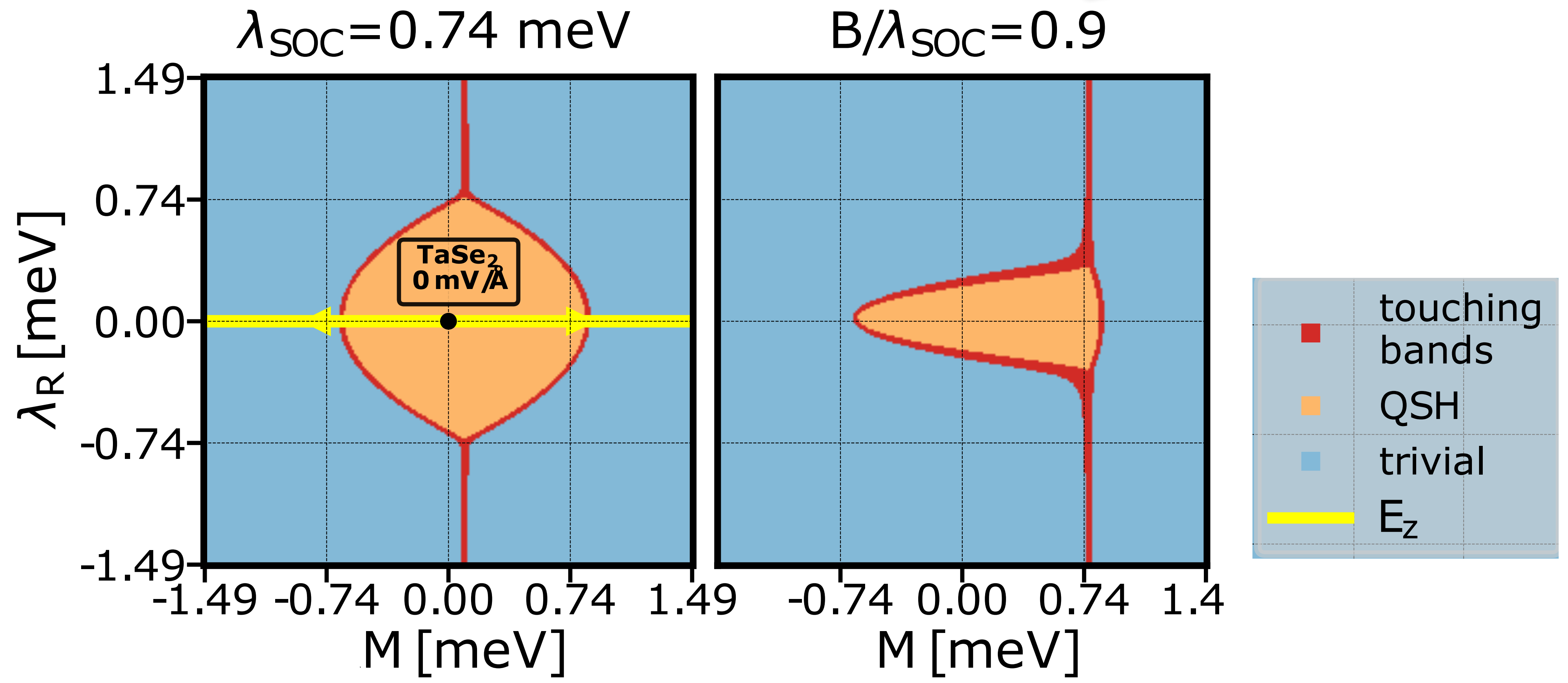
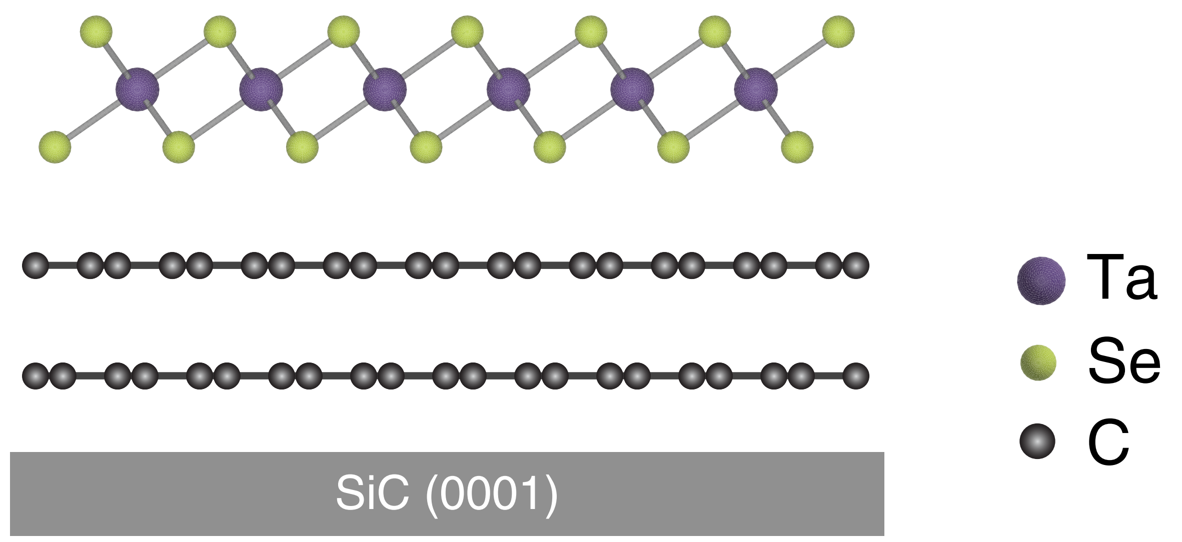
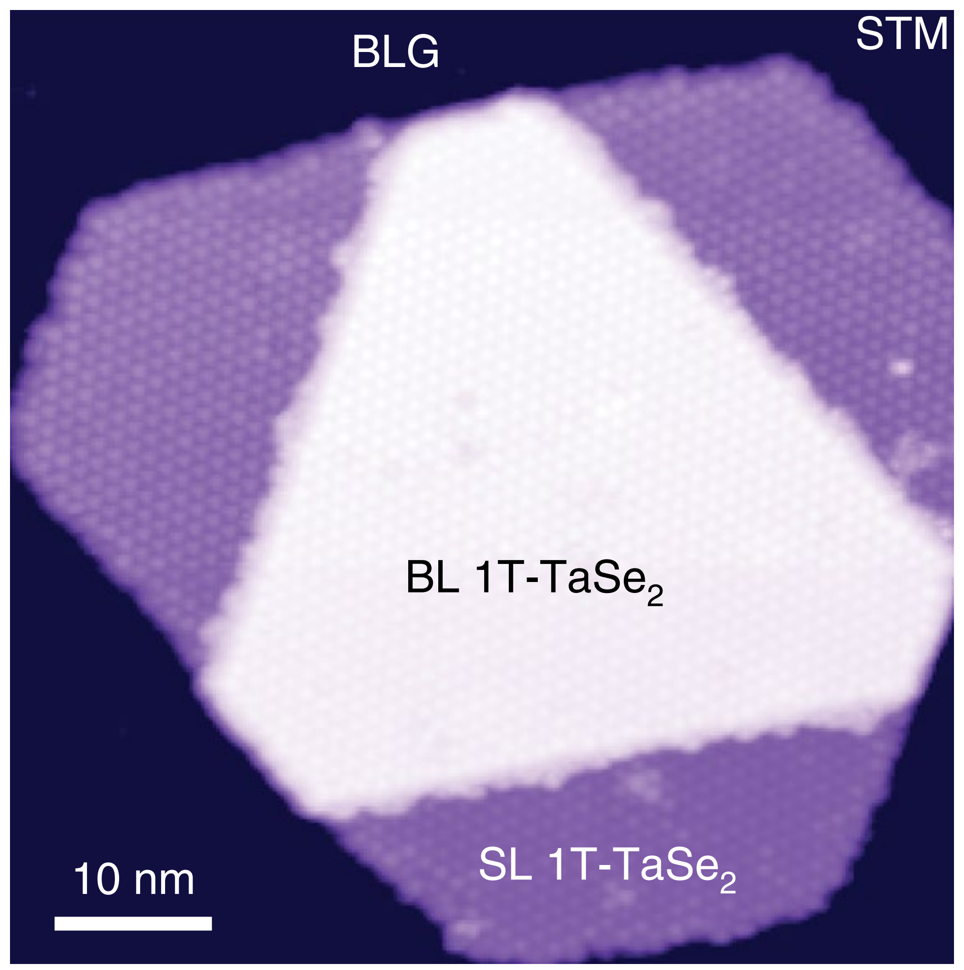


Side view





Strong correlations and orbital texture in single-layer 1T-TaSe$_2$

nature physics

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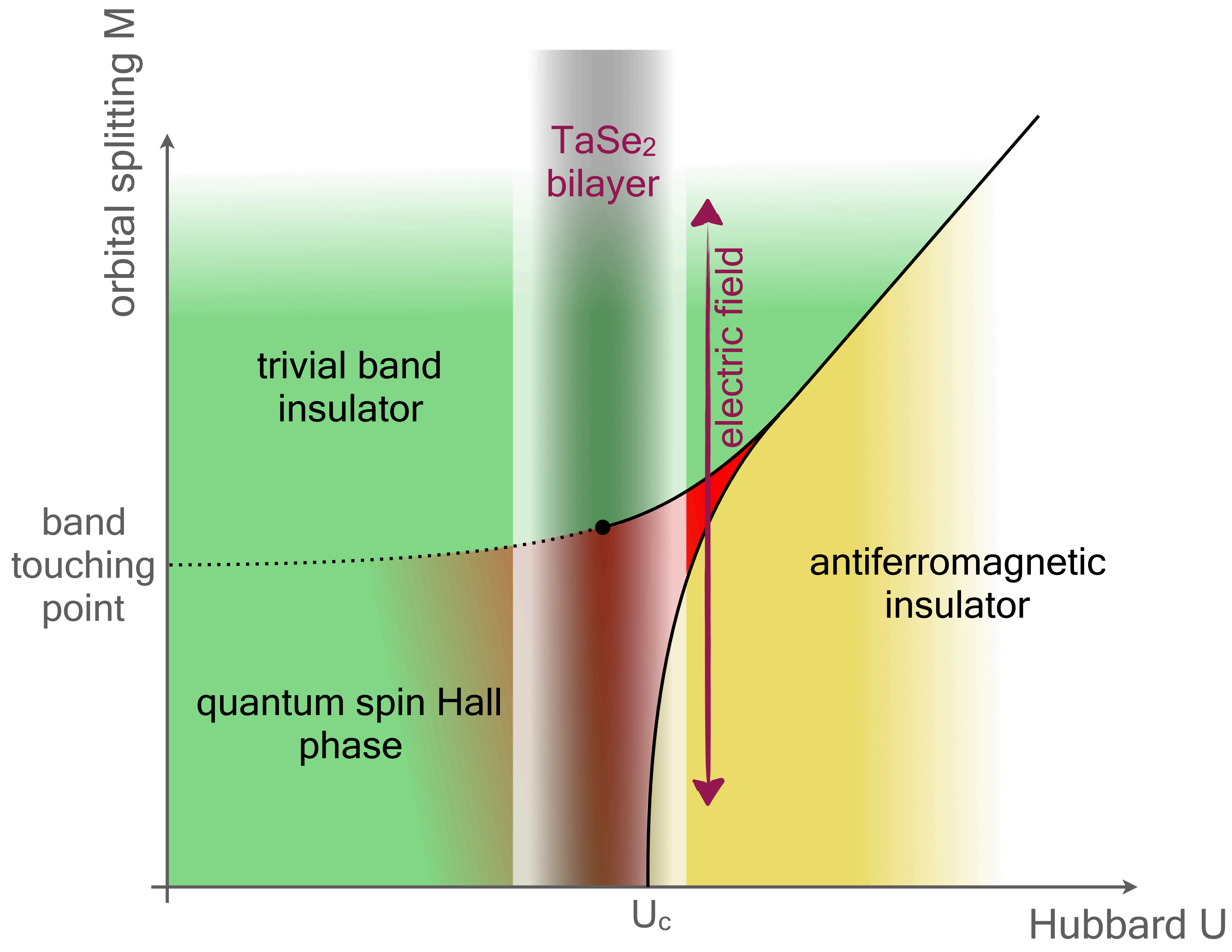
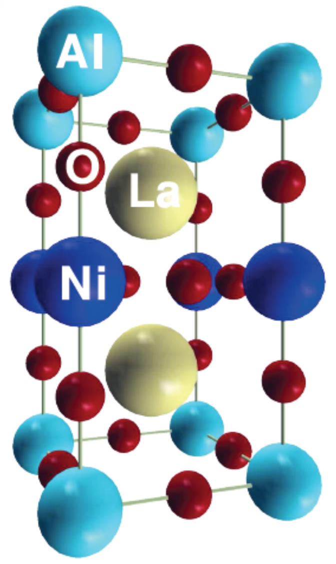
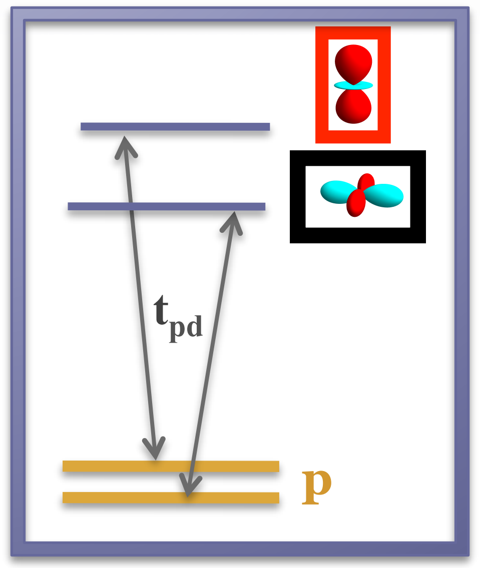
Conclusions

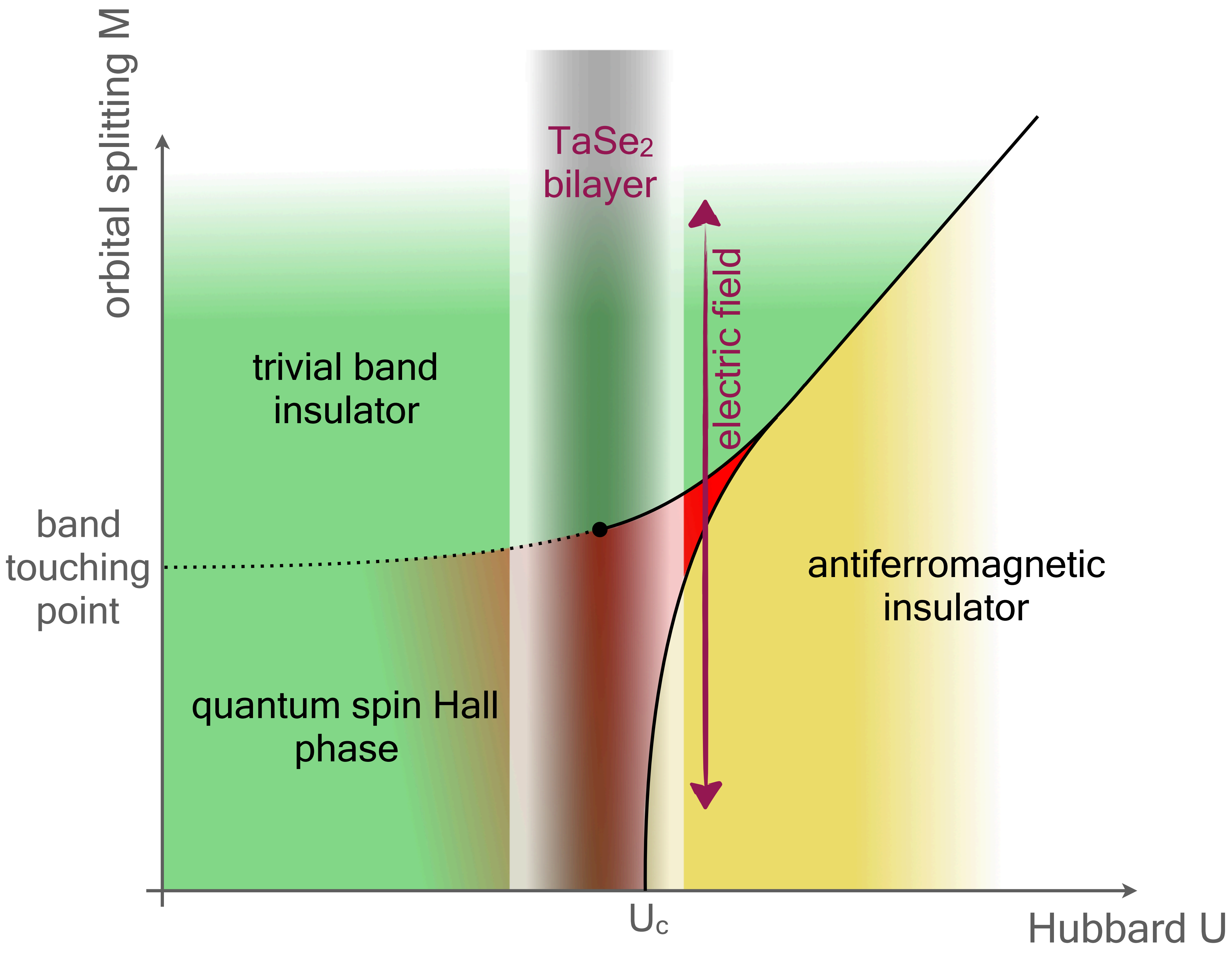


Conclusions

- many-body correction to the orbital splitting: either favoring or opposing the bare tendency







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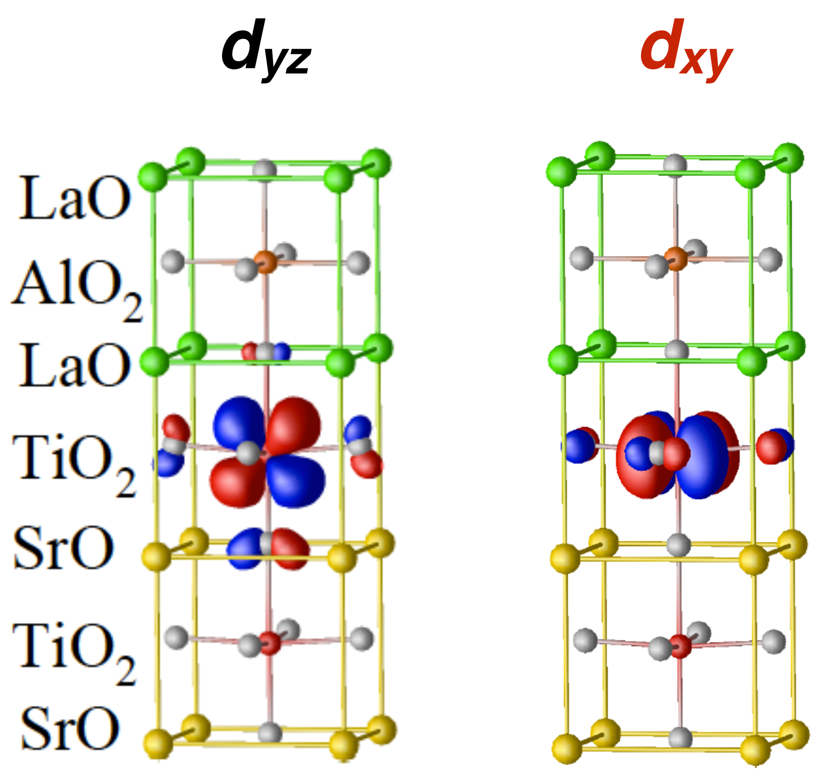
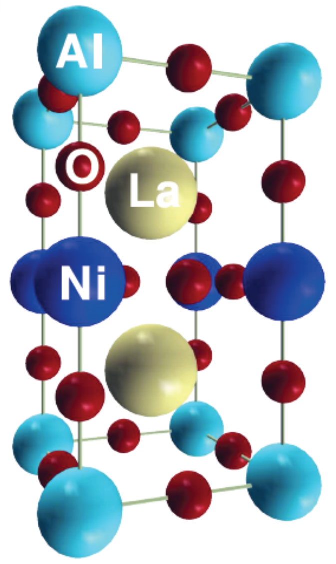
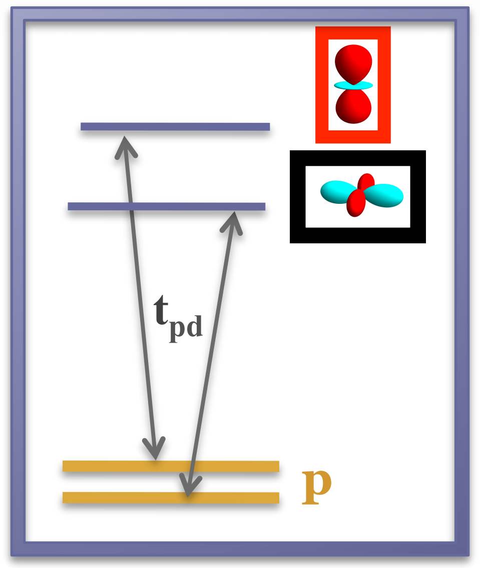
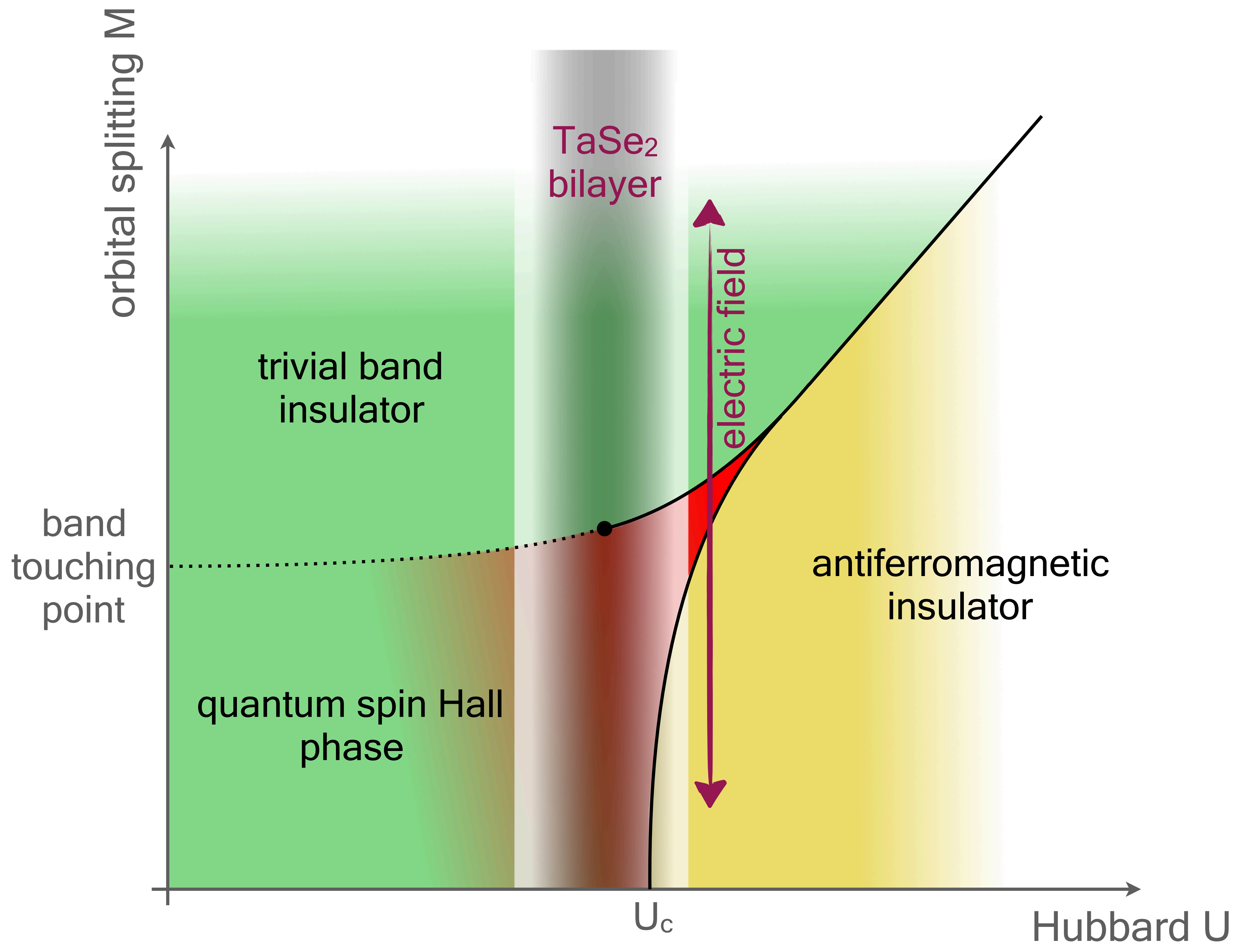






- thickness-induced metal-insulator transition in oxide heterostructures



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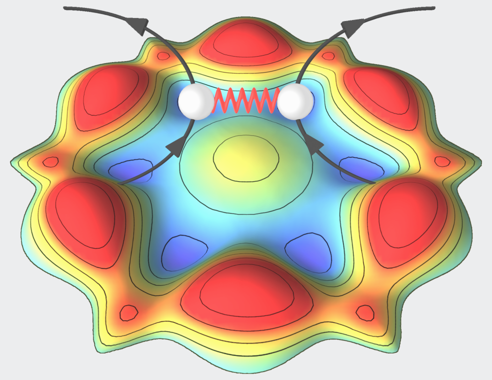

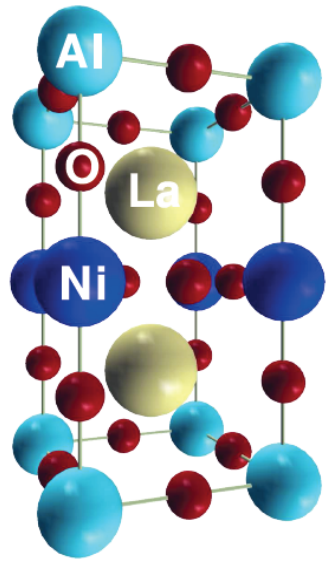

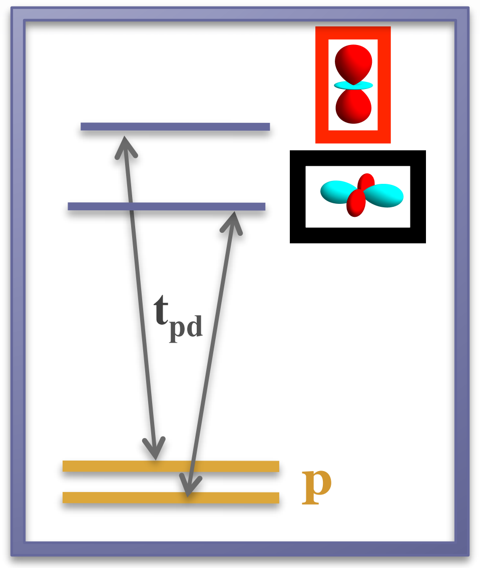

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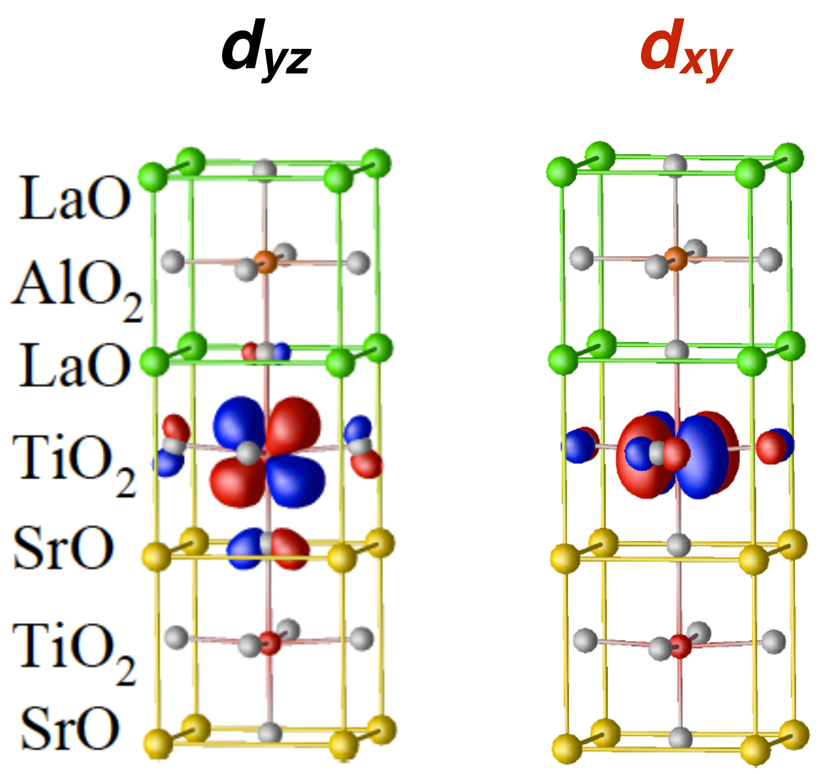

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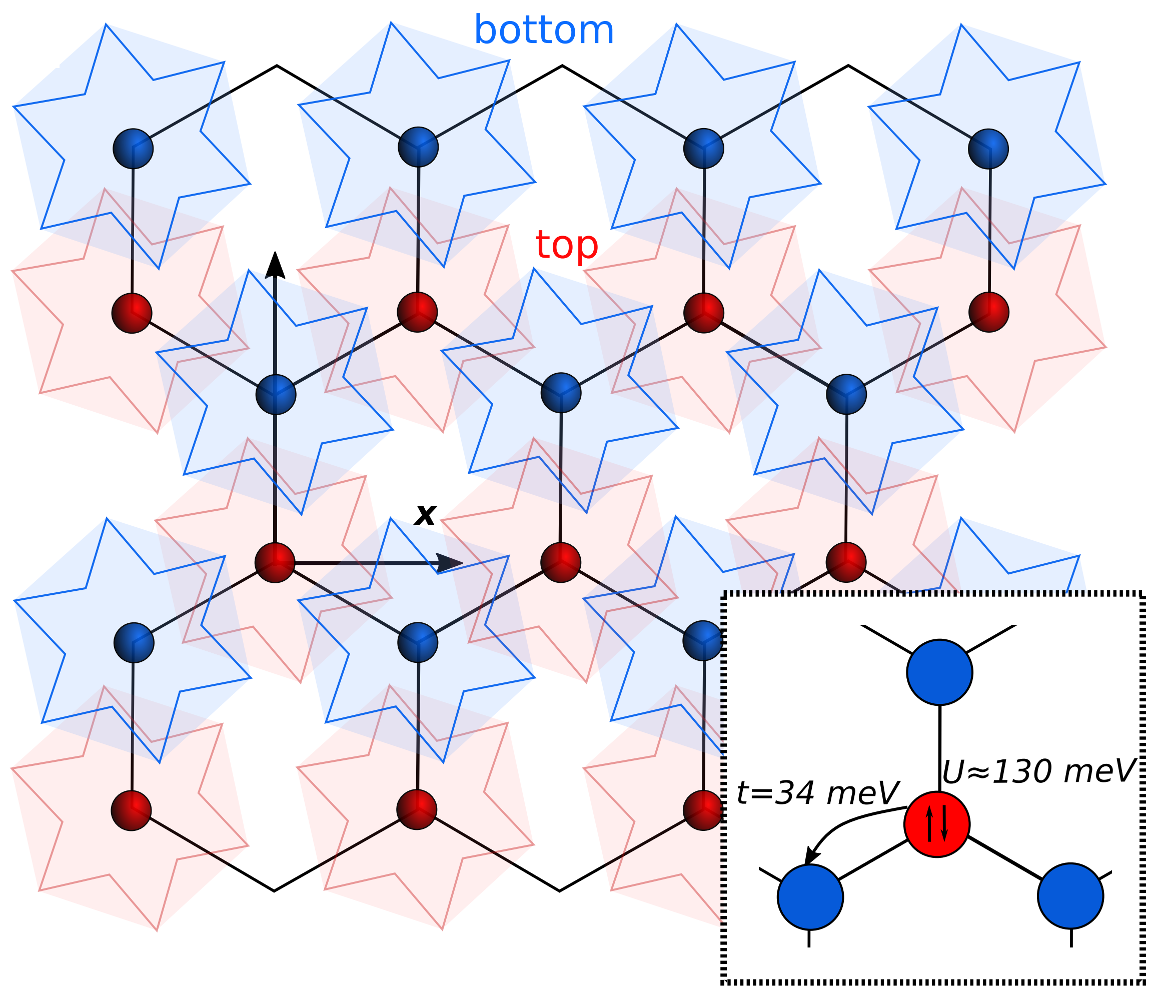
- local criticality of orbital fluctuations in correlated topological insulators



- possible material realization and tuning in transition-metal dichalcogenides