Quasiparticles in 2D with both massive and massless character

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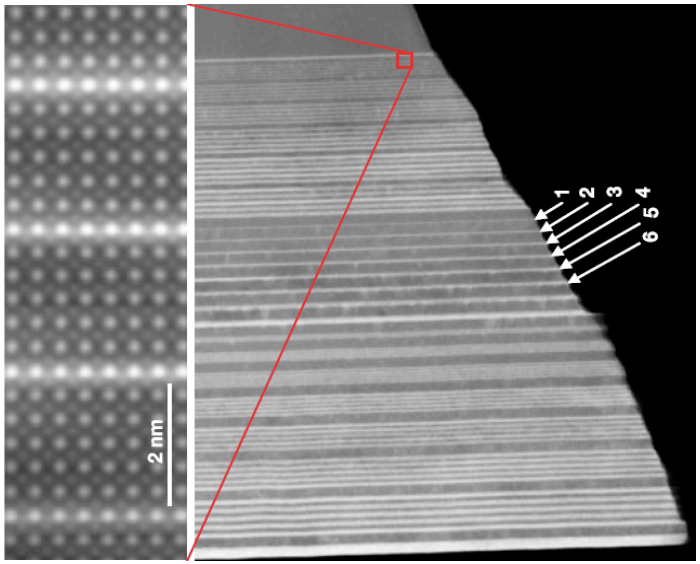
Emphases:
- Polar nature of oxides
- A new electronic state

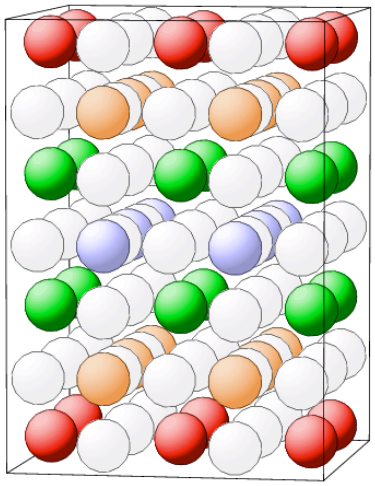
Acknowledgment: Rossitza Pentcheva, Katrin Otte (Munich)

Ionic nature locks charge in place, until…
electronic reconstruction releases tension

$LaTiO_3/SrTiO_3$ and $LaAlO_3/SrTiO_3$ heterostructures:
why are these systems so exciting?
It is due to their **polar** nature (ionicity),
which can be manipulated (within limits)
and "digital" nature (atomically layering).

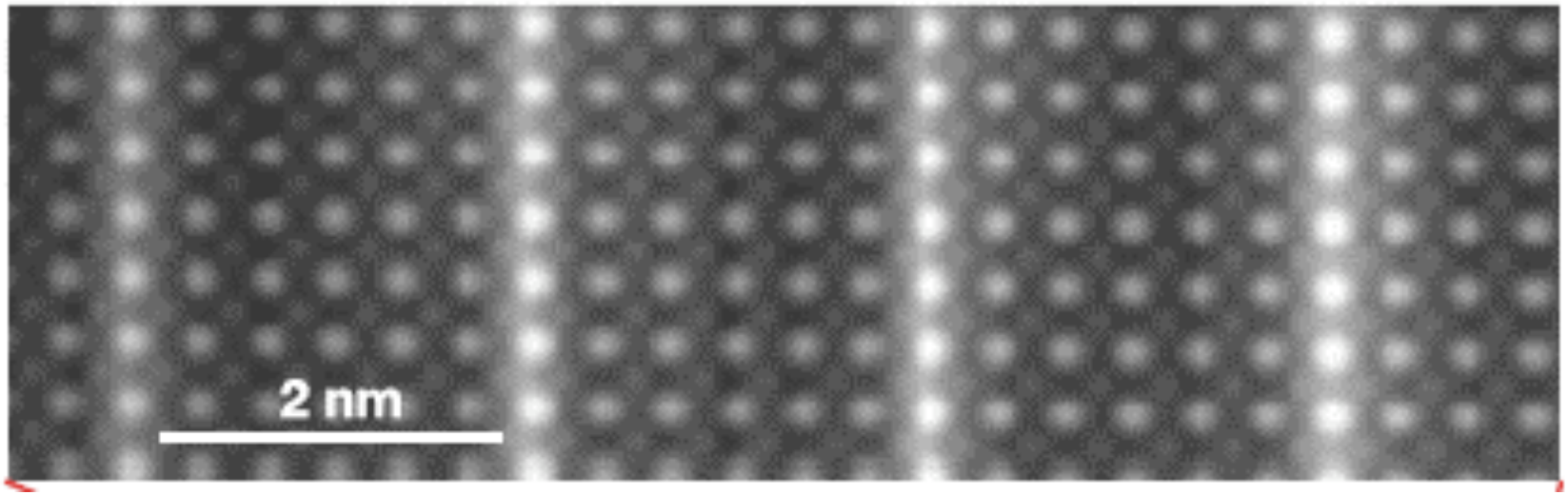


Ohtomo et al., Nature 419, 378 2002



Oxide Digital Nanostructure

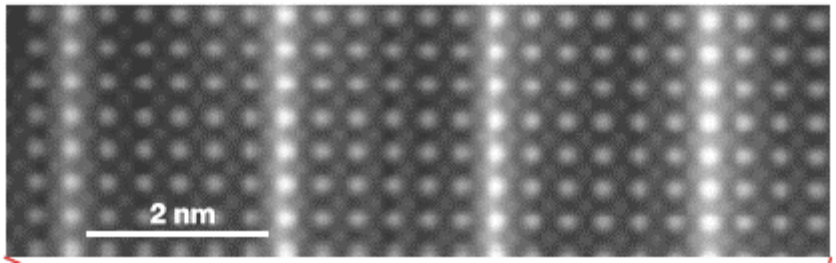
1LTO/5 STO superlattice



Ohtomo et al., Nature 419, 378 2002

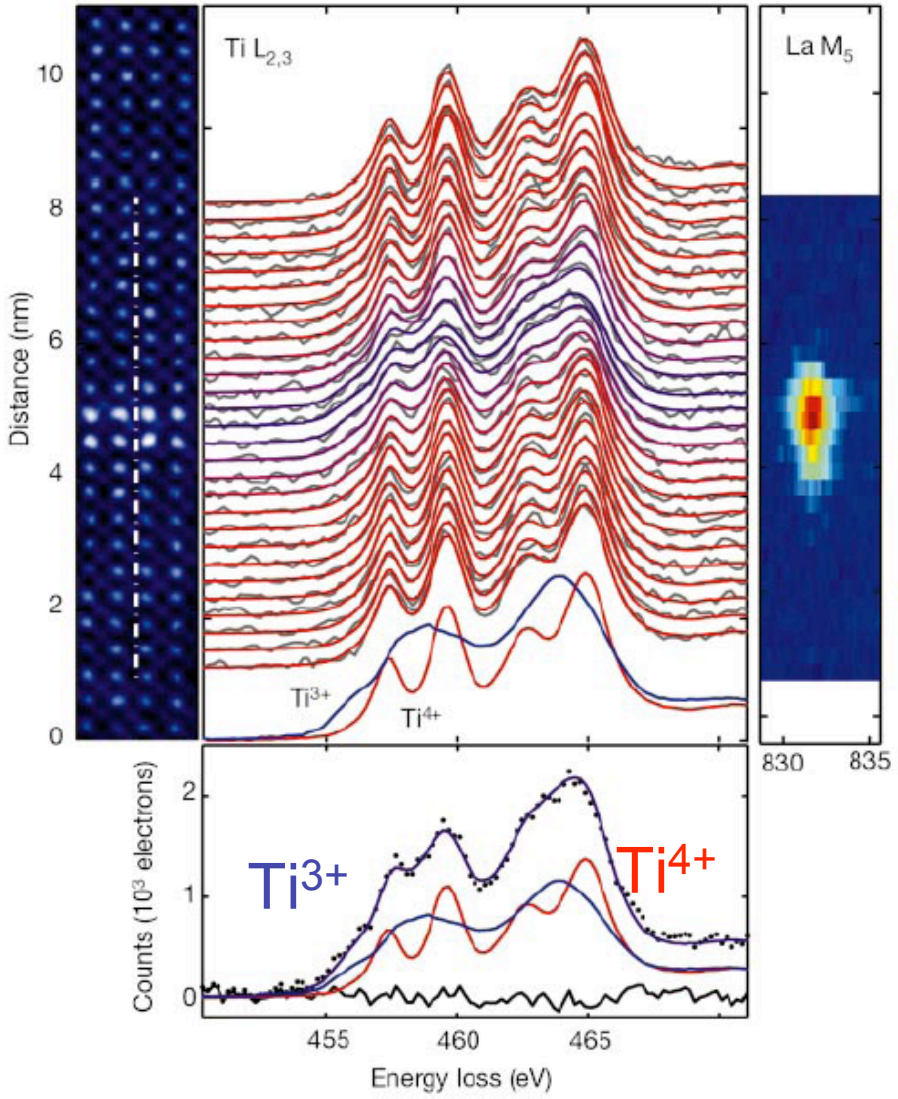
Experiments on LTO/STO superlattices

1LTO/5 STO superlattice

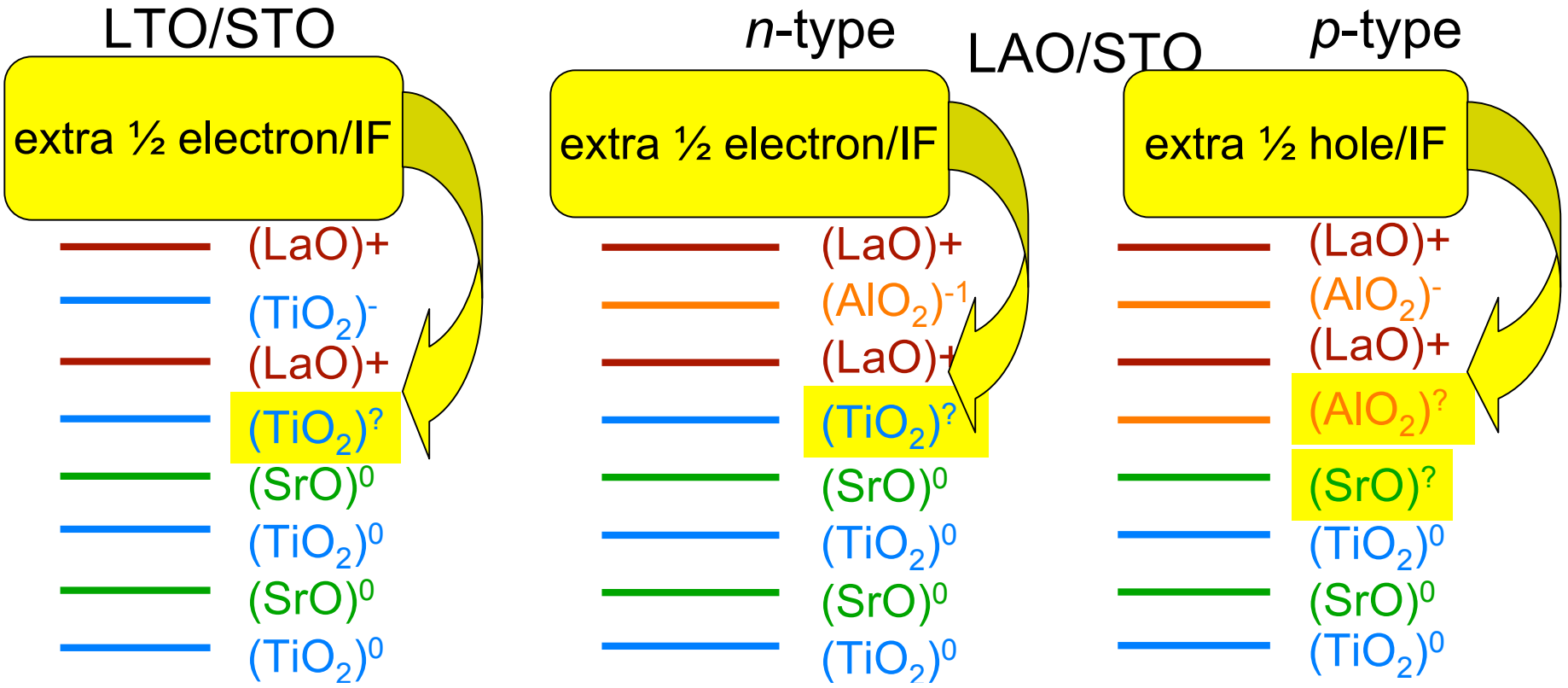


Ohtomo et al., Nature 419, 378 2002

@interface
- metallic behavior
- Ti mixed valence: 3+ and 4+.
  Specific charge states.
- length scale of charge screening: 5 STO layers



Charge mismatch@perovskite superlattices: extreme **discomfort** but no **catastrophe**



How is the charge mismatch accomodated @interface:

- insulating or conducting interface?
- novel magnetic/ charge (CO)/orbital ordering (OO)?
- can O2*p* states be correlated/magnetic?

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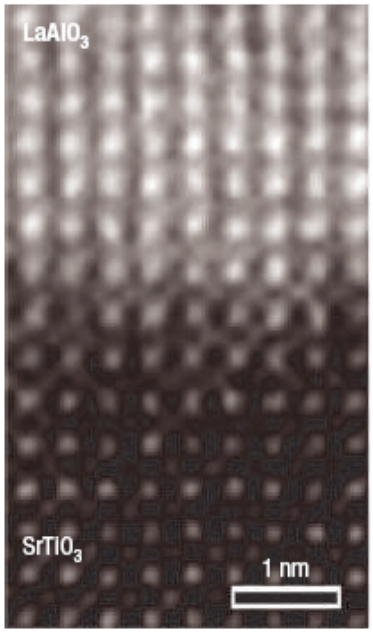
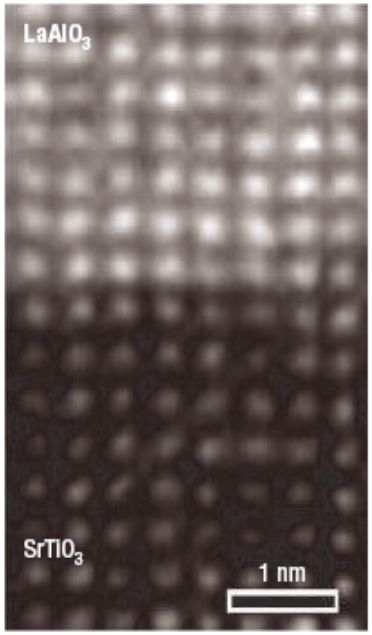
Experiments@LAO/STO IFs; important features are being understood

n-type IF: $(LaO)^{+}/(TiO_2)^{0}$



- conducting σ=1.4x$10^{-4}\Omega^{-1}$;
- high electron mobility $10^{4\text{-}5}cm^2/Vs$ [1,4],
- high carrier densities $10^{17}/cm^2$ - quasi 2DEG [1]

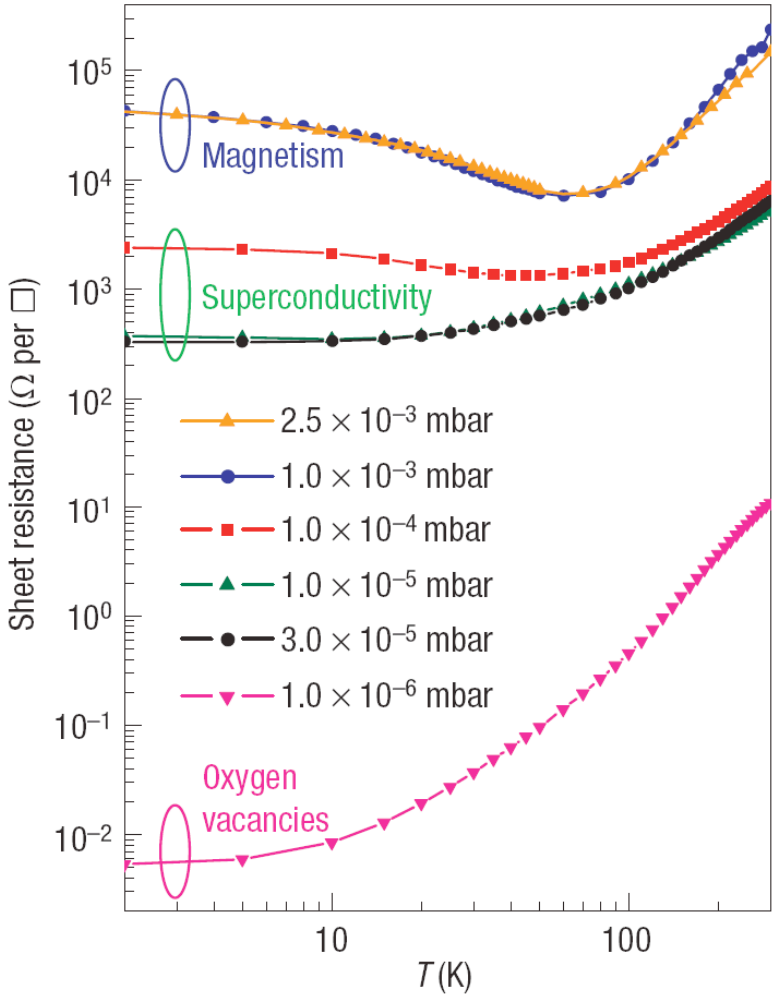
p-type IF: $(AlO_2)^{-}/(SrO)^{0}$



- insulating, $\sigma=10^{-7}\Omega^{-1}$
- structurally ideal IF[1]/defects [2]

[1] Ohtomo and Hwang, Nature 427, 423 (2004)
[2] Nakagawa, Hwang&Muller, Nat. Mat. (2006)
[3] Huijben et al., Nat. Mat. (2006).
[4] S. Thiel et al., Science 313 (2006).

The *n*-type LAO/STO IF: oxygen pressure



(Rijnders&Blank, Nat. Mat. 2008)

- magnetism
(Brinkman et al, Nat. Mat. 2007)

- superconductivity
(Reyren et al, Science 2008)

- conductivity
(Ohtomo&Hwang, Nature 2004)

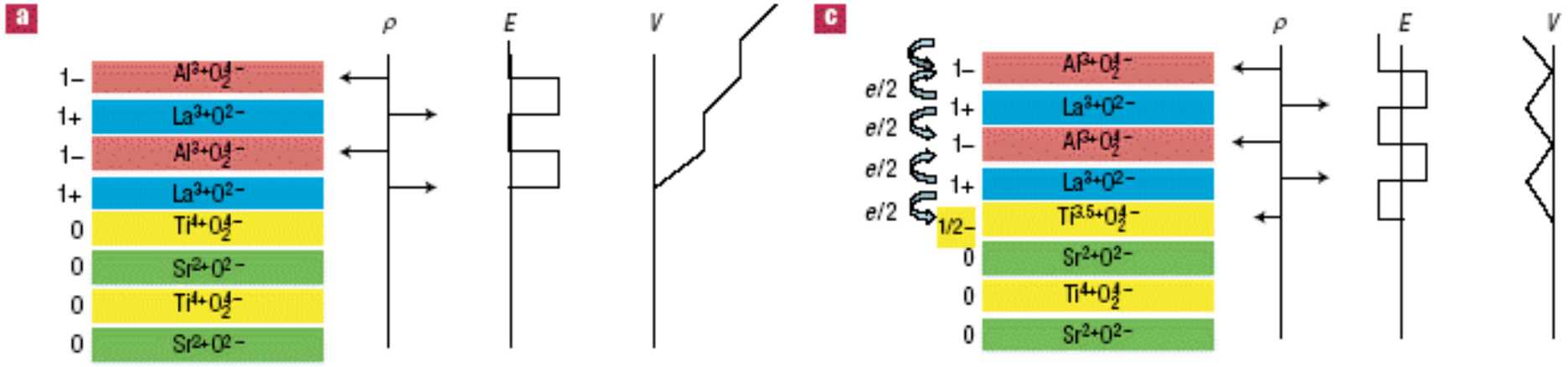
Role of p_{O2}:
(Nakagawa, Hwang&Muller, Nat. Mat. (2006),
Herranz et al., PRL 2007,
Siemons et al., PRL 2007,
Kalabukhov, PRB R, 2007)

LAO slab on STO substrate

- Perovskite superlattices
  - $LaAlO_3/SrTiO_3$: the n-type interface
- $LaAlO_3$slab on $SrTiO_3$(001) substrate:
  surface coupled to an interface

The Polarization Catastrophe

Adding a slab of polar material on a nonpolar (different) material.

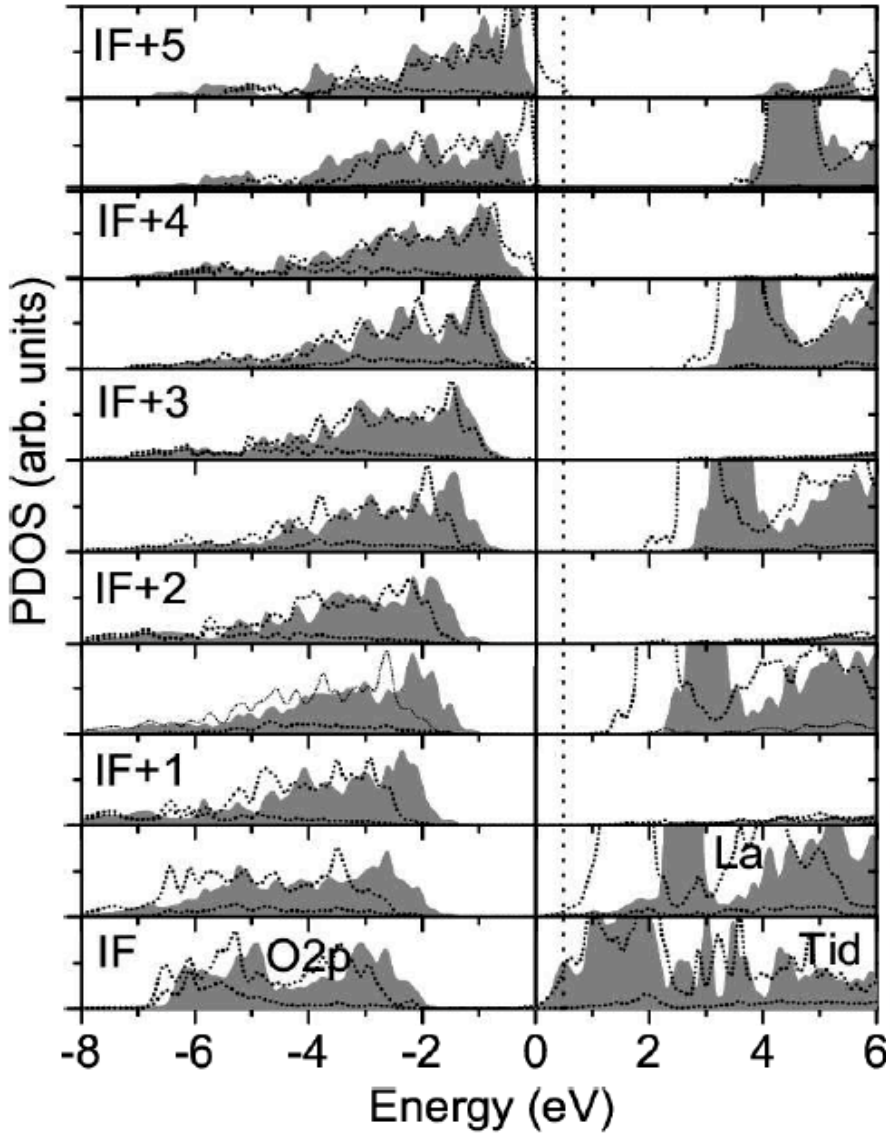


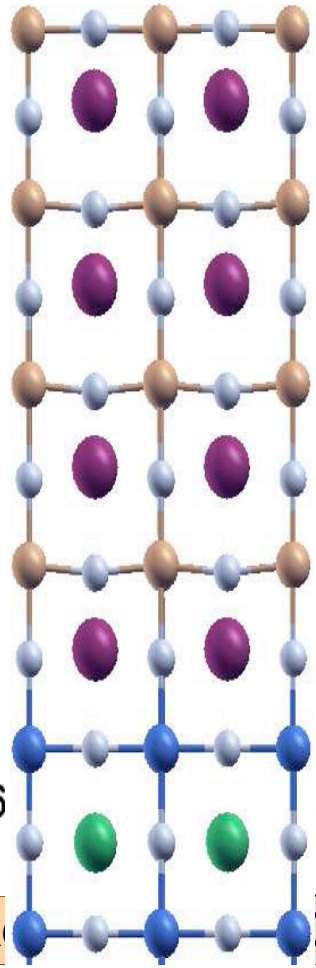
- Nakagawa et al., Nature Mat. (2006)

Five layers of $LaAlO_3$ on $SrTiO_3$ leads (in a purely rigid ionic picture) to a potential difference from substrate to surface of ~100 eV.

This is nonsense of course: the band gap of $LaAlO_3$ is 5.6 eV.
So what is the real story? (extpl & theory)

5ML LAO/STO(001) surfaces: band alignment





Upward 'ramp' shift of O 2p bands layer-by-layer

Ideal positions: metallic behavior with partial occupation of Ti 3d states@IF

Relaxed structure:
VBM determined by O2*p*@surface
CBM by Ti *3d* states @ IF;
Ti remains in 4+ state

Next:
electronic reconstruction

rutile TiO_2/VO_2 (001) heterostructures

TiO_2/VO_2 (001) is Ti^{4+} - V^{4+} [d^0 - d^1 system] of a band ins., peculiar Mott-Peierls ins.

No polar discontinuity; is it boring?

VO_2 is a strongly correlated system with a metal-insulator transition at 340 K

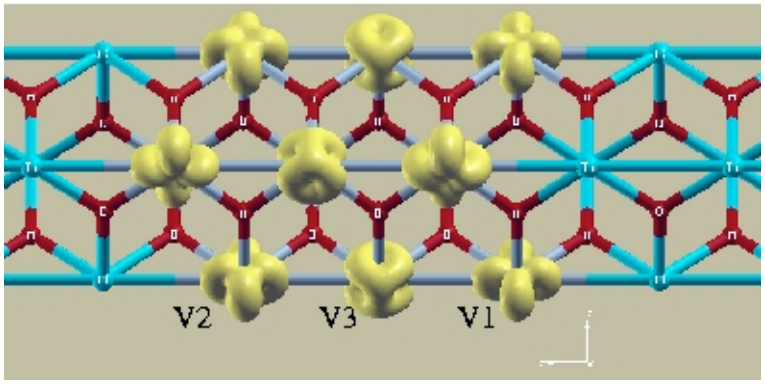
rutile TiO_2/VO_2 (001) heterostructures

Synthesis and Characterization of TiO_2/VO_2 multilayers

Dan Lam's group, ANL (1990-93). Coherent TiO_2/VO_2 interfaces
Muraoka, Hiroi, APL 2002. Tuning of VO2 metal-insulator transition
Okazaki, Sugai, Muraoka, Hiroi, PR B 2006. PES study of spectral weight
Maekawa PR B 2007. PES study of conducting vs insulating interface
Nagashima, Yanagida, Tanaka, Kawai, JAP 2007. 5 nm required for MIT

Superlattice: $(VO_2)_3/(TiO_2)_5$

1 electron on each V ion

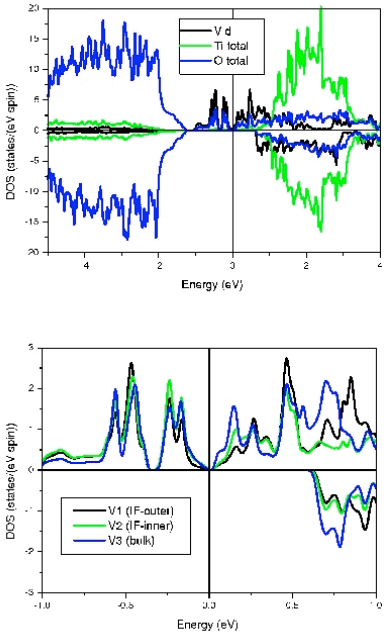


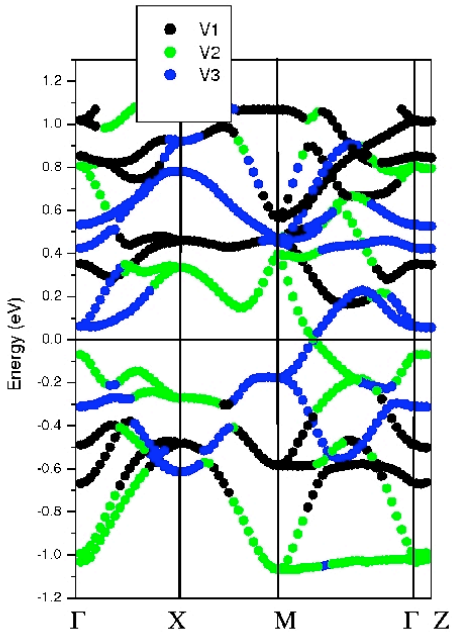
So, interesting but unexciting, right?

Wrong. Unusual electronic structure.

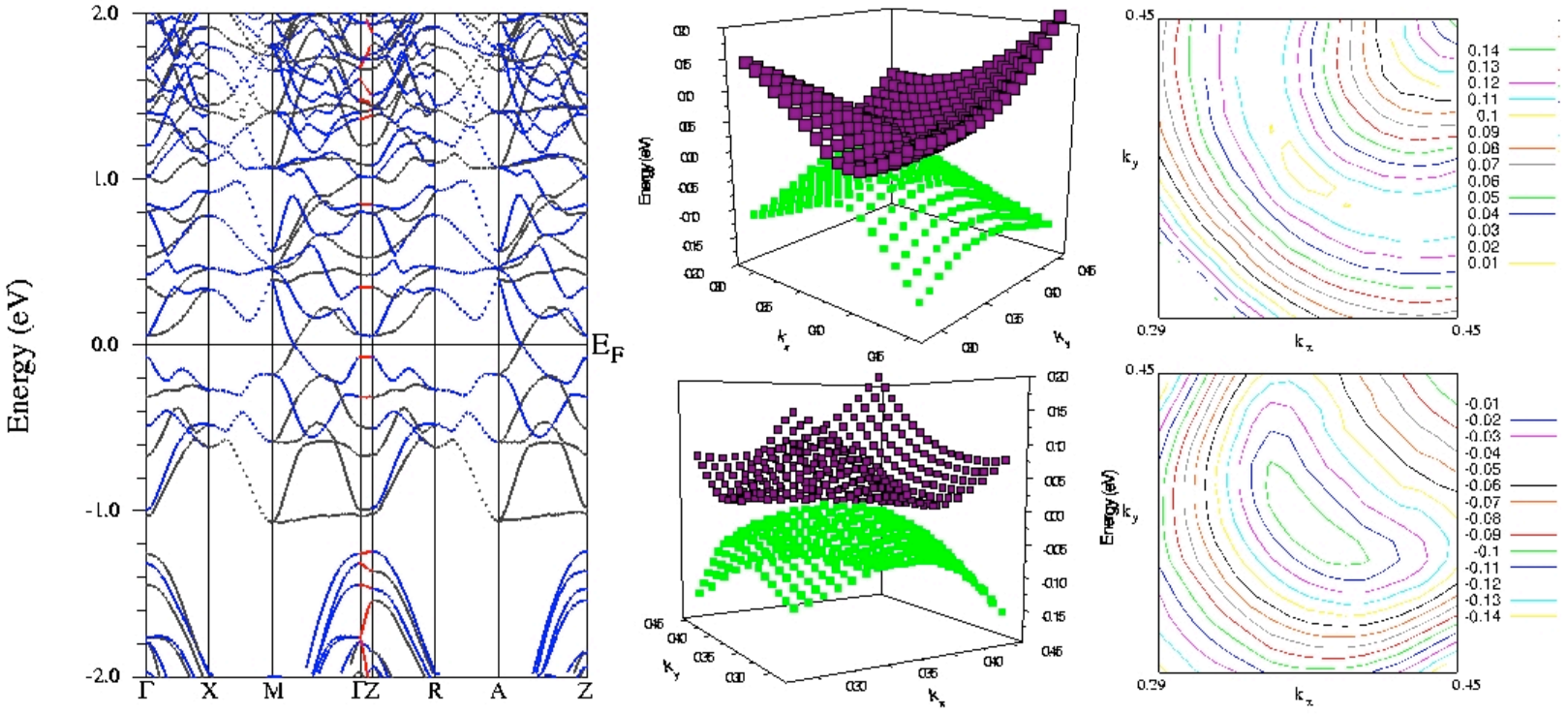
3 unit cells of VO_2 encased within TiO_2.

- only small atomic relaxation from ideal
- unexpected V 3d orbital ordering
- half metallic 2D slab





"semiDirac" phase in 2D VO_2 trilayer



Point Fermi surface; E(k) = $+/-[(k_x^2/2m^*)^2 + (vk_y)^2]^{1/2}$

"massive" along x' (particle-like), "massless" along y' (photon-like).

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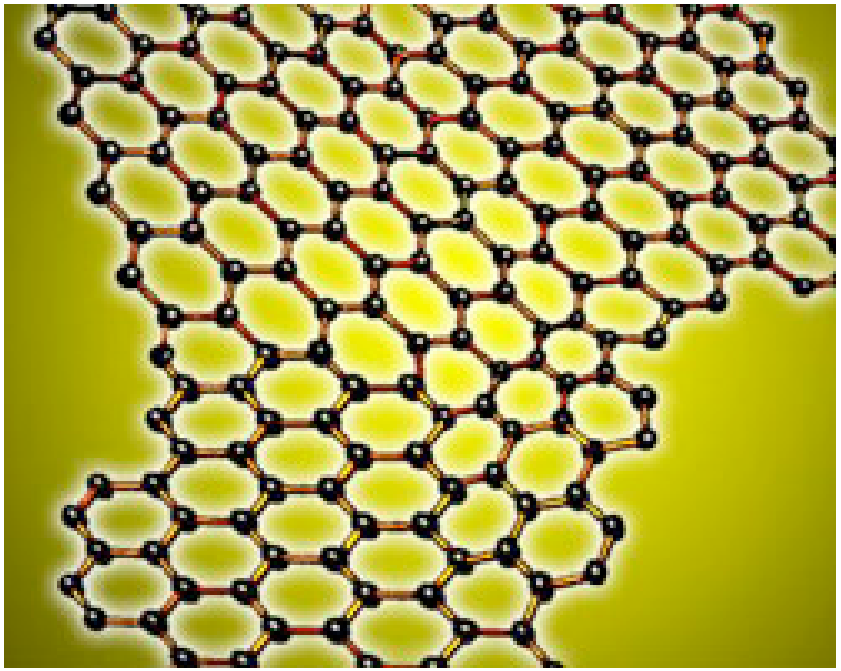
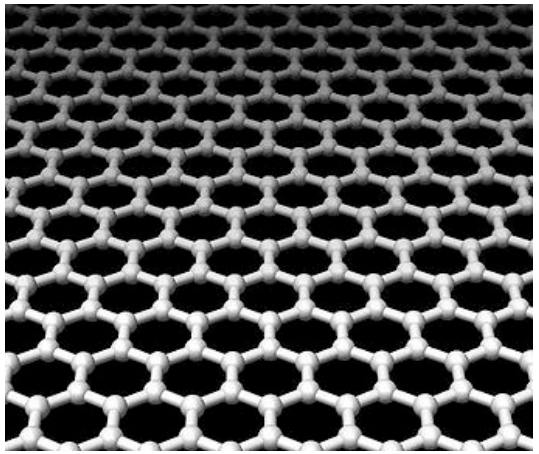
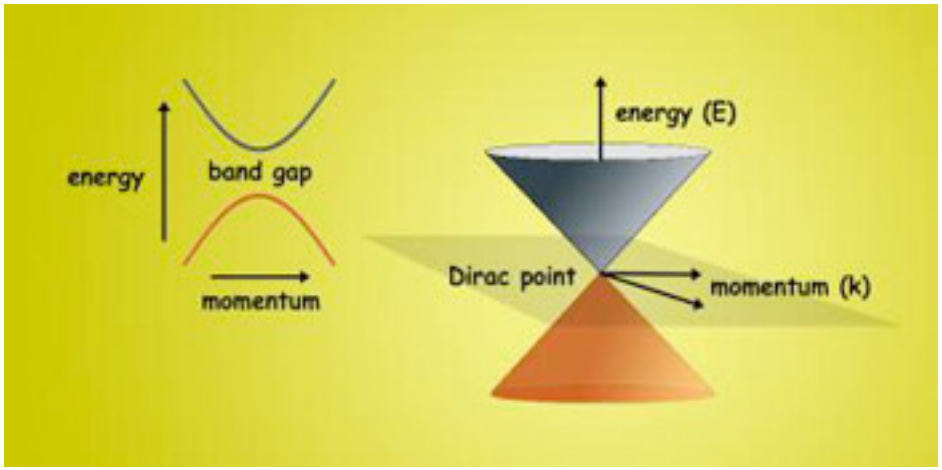
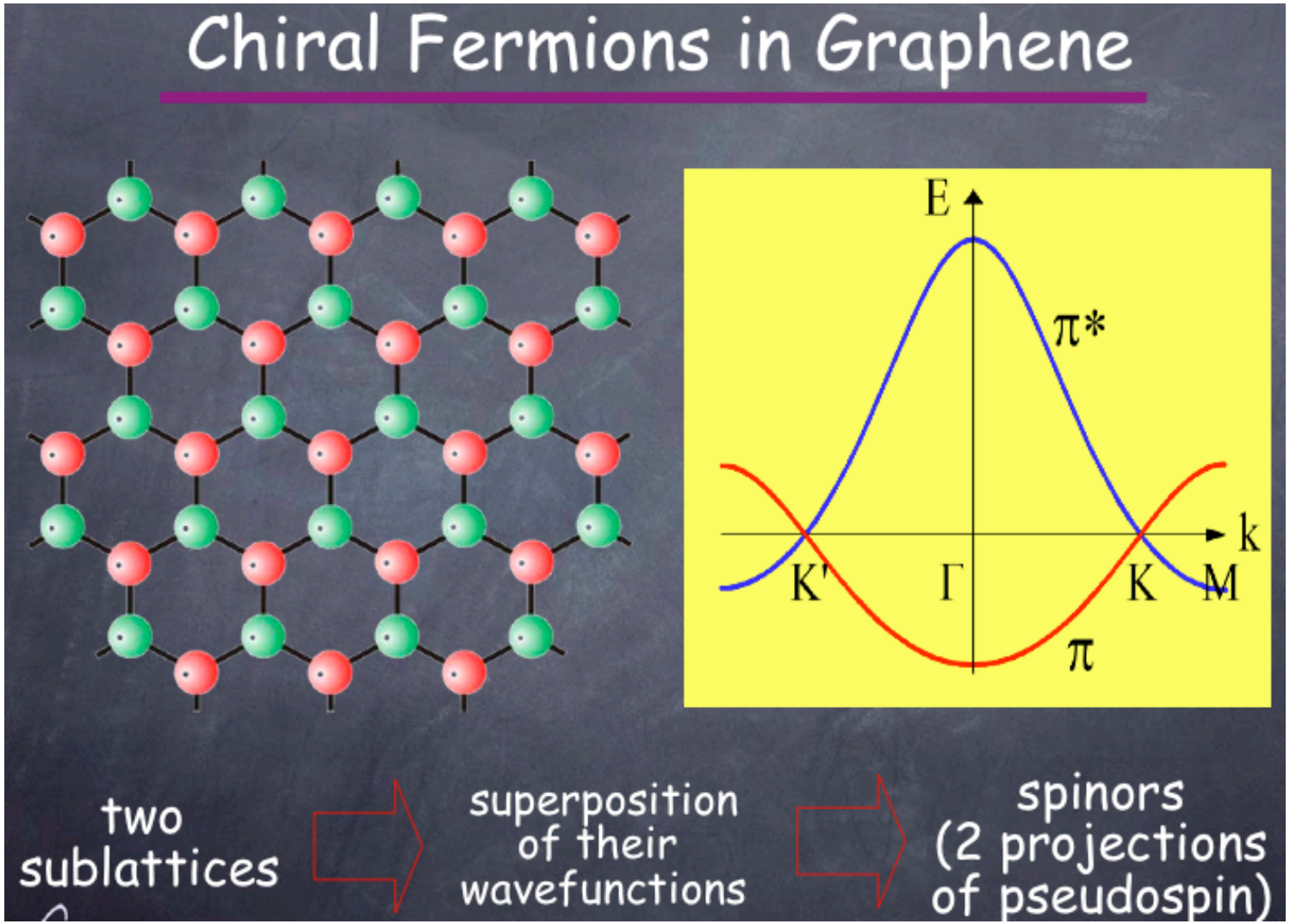
Graphene: single layer graphite





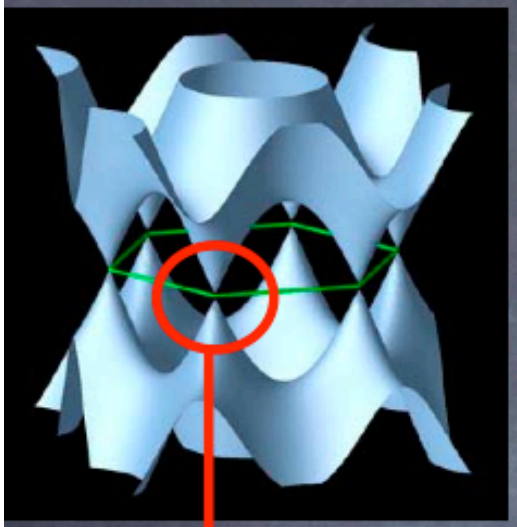


Graphene basics



Electronic structure of graphene

Dirac fermions in graphene

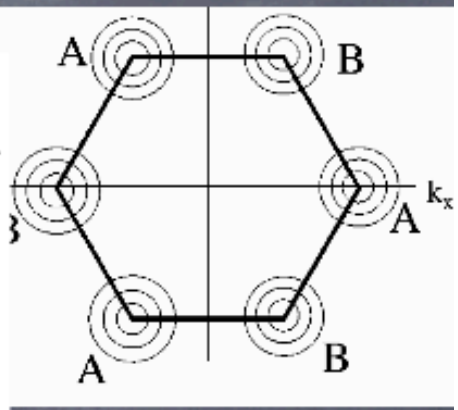


$$K.E. = \pm v\,|P|$$

$$K.E. = \pm\sqrt{m^2v^4 + v^2P^2}$$

$$m = 0$$

$$v \approx c/300$$

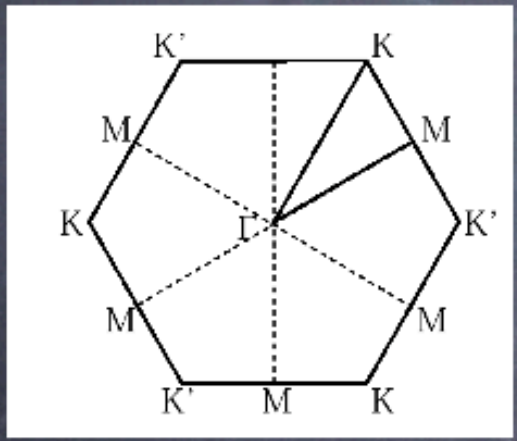


Low energy elementary excitations are two-dimensional Dirac-Fermions.

DOS is similar top d-wave SC because of nodal points

Dirac Fermions in Graphene

Brillouin zone

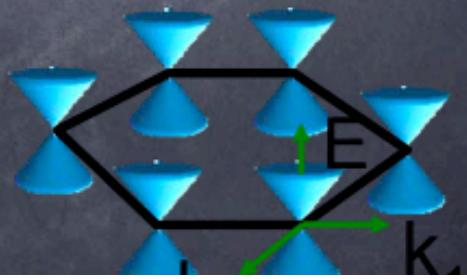


Tight binding model

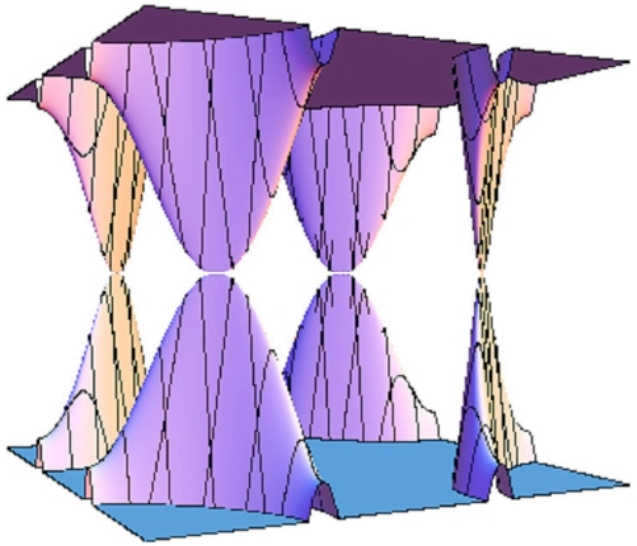
$$H_k = \begin{pmatrix} 0 & \xi(k) \\ \xi^*(k) & 0 \end{pmatrix}$$

$$\xi(k) = t\sum_{j=1}^{3} e^{ik(b_j - b_1)}$$

$$H_{K\pm} = v_f\hbar(k_1\sigma_1 \mp k_2\sigma_2)$$



Four semiDirac points along (1,1) directions in the square Brillouin zone



Minimal model for semiDirac system:

* Orbital A: $E_1 + 2t[\cos k_x + \cos k_y]$
* Orbital B: $E_2 - 2t[\cos k_x + \cos k_y]$
* Orbital C: E_3, distant in energy

Coupling A-C, B-C (not A-B):

$2t' [\cos k_x - \cos k_y]$

$$H = \begin{pmatrix} \varepsilon_1 + 2t(\cos k_x + \cos k_y) & 0 & 2t'(\cos k_x - \cos k_y) \\ 0 & \varepsilon_2 - 2t(\cos k_x + \cos k_y) & 2t'(\cos k_x - \cos k_y) \\ 2t'(\cos k_x - \cos k_y) & 2t'(\cos k_x - \cos k_y) & \varepsilon_3 \end{pmatrix}$$

Result: four semiDirac points along the four (1,1) directions

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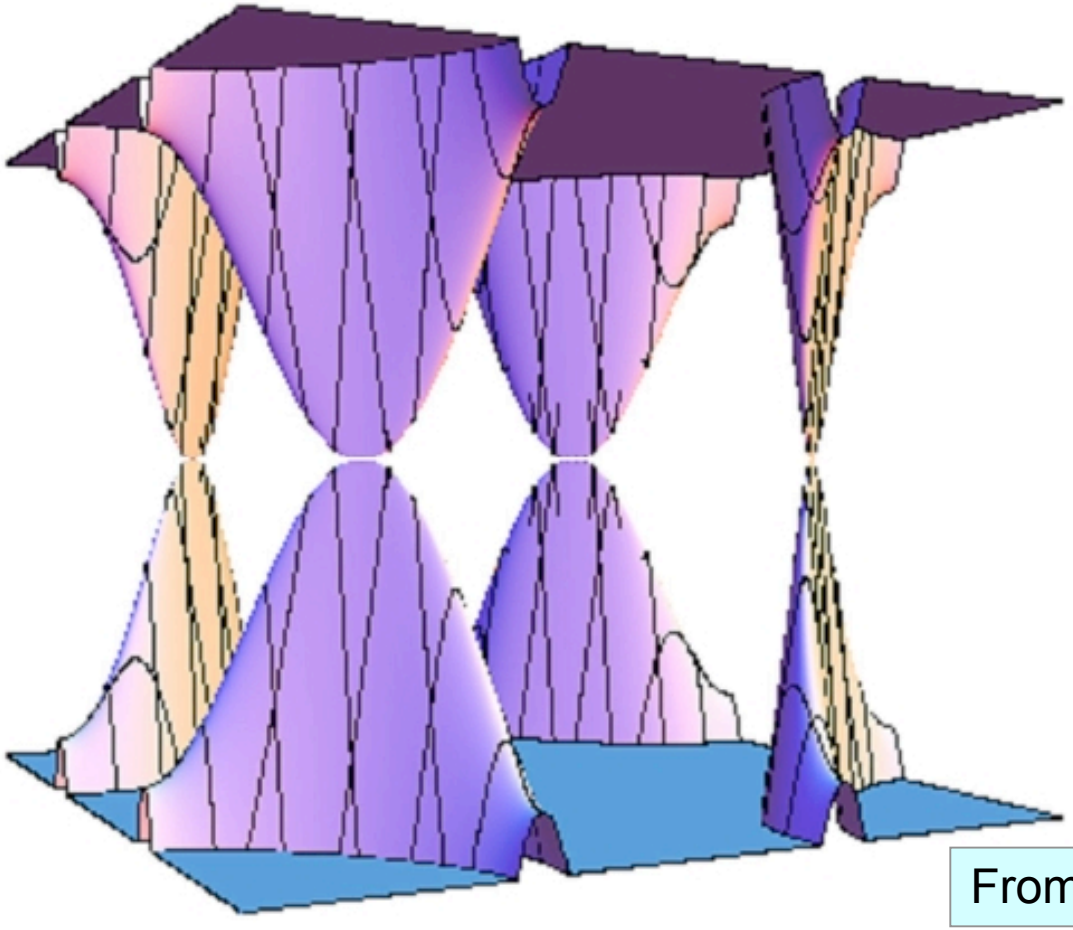
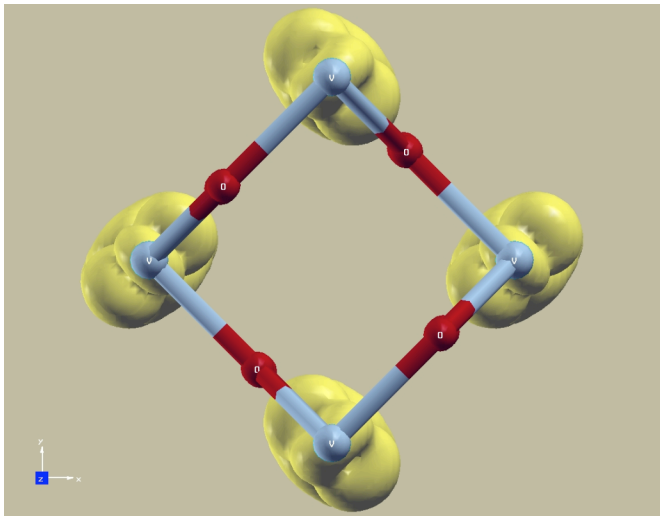
Four semiDirac points along (1,1) directions in the square Brillouin zone

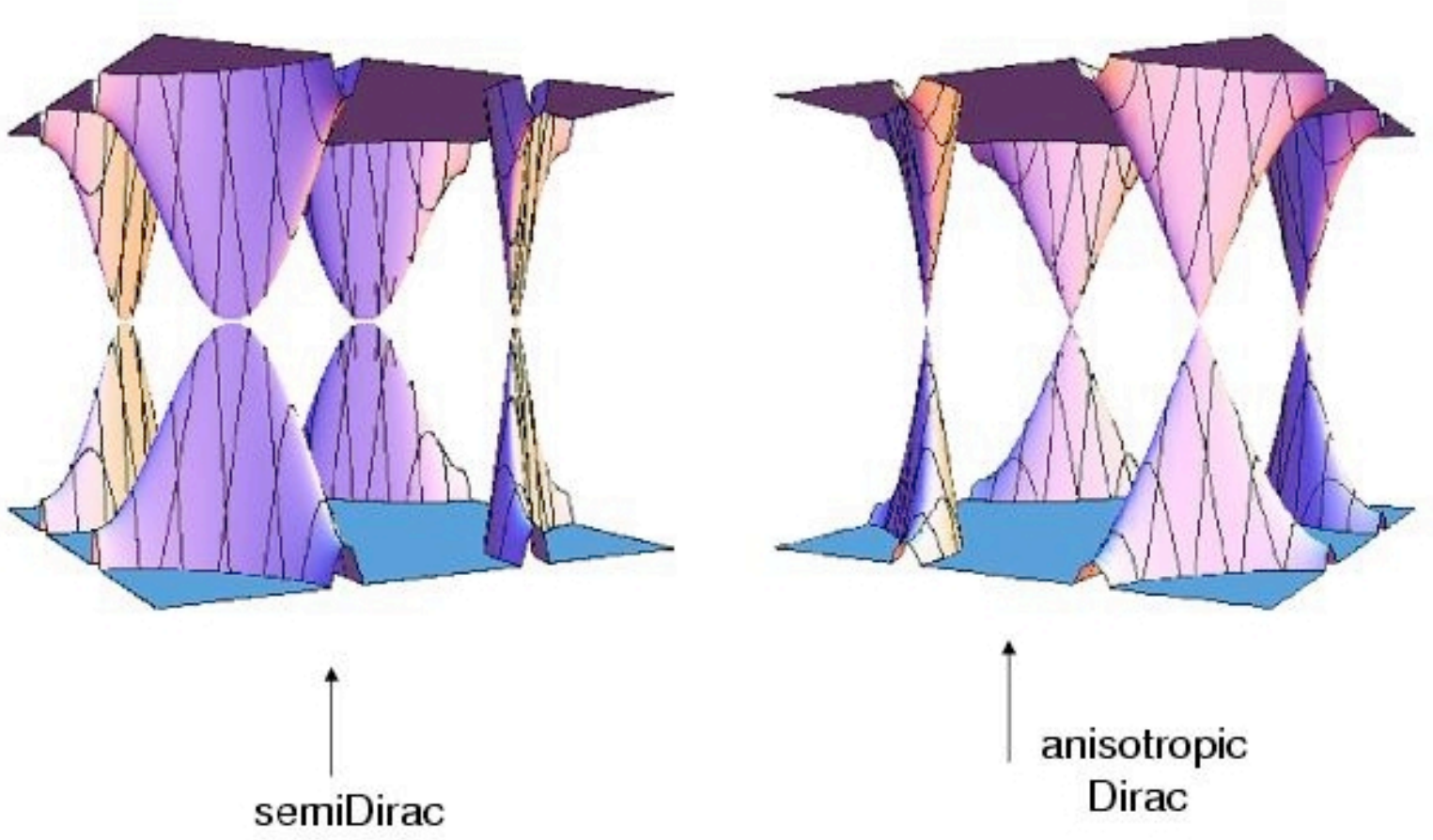




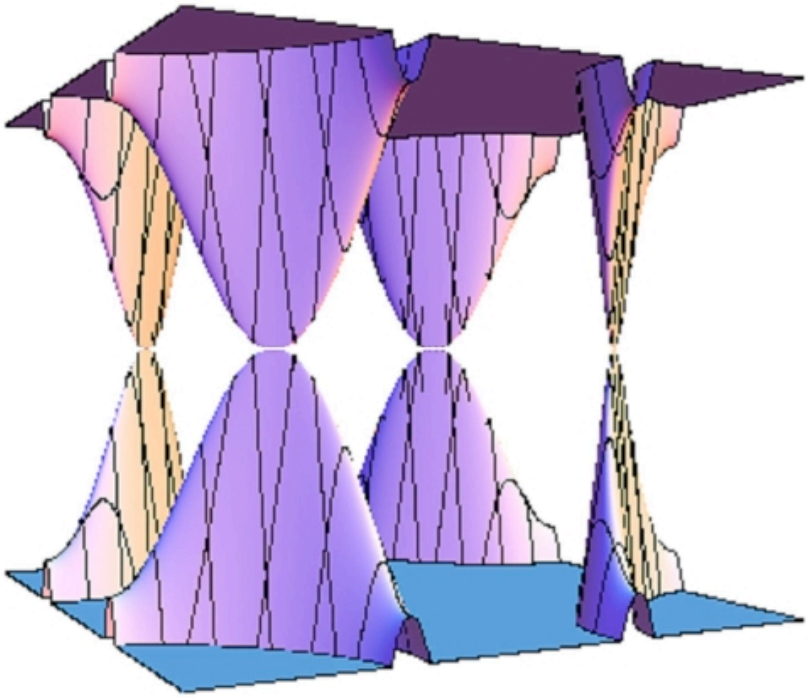
Looking down on the VO_2 trilayer spin density

From the tight-binding model

Comparison: semiDirac to anisotropic Dirac



Electrons in a semiDirac system, "semiDirac quasiparticles"



usual 2D: N(E) ~ constant

semiDirac: N(E) ~ $|E|^{1/2}$

Dirac: N(E) ~ |E| (graphene)

semiDirac N(E) is non-analytic, has higher DOS near the point Fermi surface than Dirac system

different behavior in a magnetic field; (presumably) different QHE and associated edge states

Magnetic field

Point Fermi surface; $E(k) = +/- \sqrt{[(k_x^2/2m^*)^2 + (vk_y)^2]}$
massive along x', massless along y'

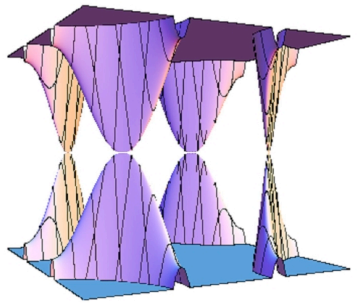
The low energy Hamiltonian for the two bands is

$$H = \begin{bmatrix} p_x^2/2m & vp_y \\ vp_y & -p_x^2/2m \end{bmatrix}$$

Then p --> p-(e/c)A to treat field. The cyclotron harmonic oscillator potential becomes an asymmetric quartic potential in the semiDirac problem. New behavior will emerge.

Summary: semiDirac quasiparticles

A new "semiDirac" quasiparticle state in the TiO_2/VO_2 (001) system due to quantum confinement + appropriate ionic configuration



Features compared to graphene:

- half metallic (no spin degree of freedom) rather than spin-degenerate
- semiDirac spectrum rather than Dirac spectrum
- distinct quantum Hall/spin quantum Hall behavior is displayed
- point FSs along (1,1) directions, not at fixed symmetry points
- each point is "maximally anisotropic" rather than isotropic
- solid state heterostructure is robust, graphene is flexible
- heterostructure can be etched to study edge states, shape effects
- TB model gives real possibility of design of other semiDirac systems

+ -	dipole= - a
+ - + -	dipole= -2a
+ - + - + -	dipole= -3a
+ -	dipole= - a
- + - +	dipole= +2a
+ - + - + -	dipole= -3a