

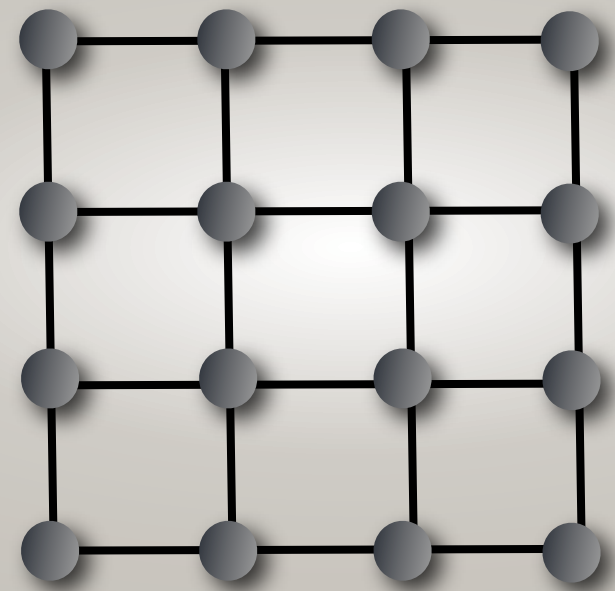


# Naval Research Laboratory

## Theoretical Perspective on Iron Pnictide Superconductivity

Michelle Johannes

Igor Mazin  
David Singh  
Devina Pillay

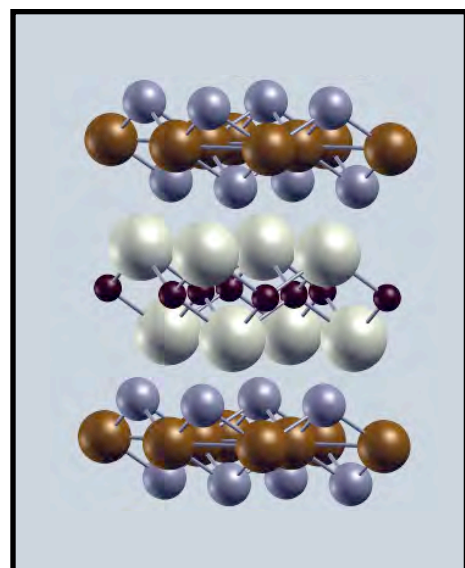




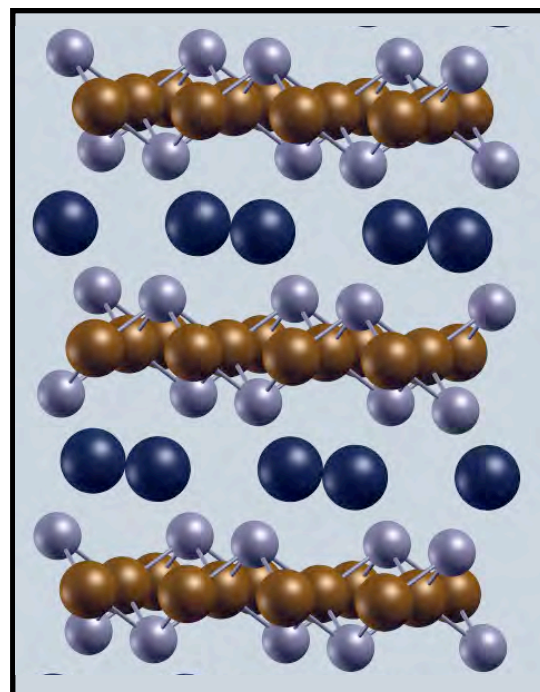
# Structural Types

Parent compounds:

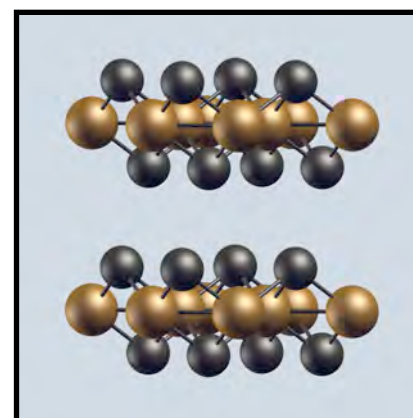
1111 (LaOFeAs)



122 (BaFe<sub>2</sub>As<sub>2</sub>)



11 (FeTe)



Also:  
LiFeAs, SrFeAsF  
(111)

22K LaO<sub>0.9</sub>F<sub>0.1</sub>FeAs

27K FeSe

38K Ba<sub>0.6</sub>K<sub>0.4</sub>Fe<sub>2</sub>As<sub>2</sub>

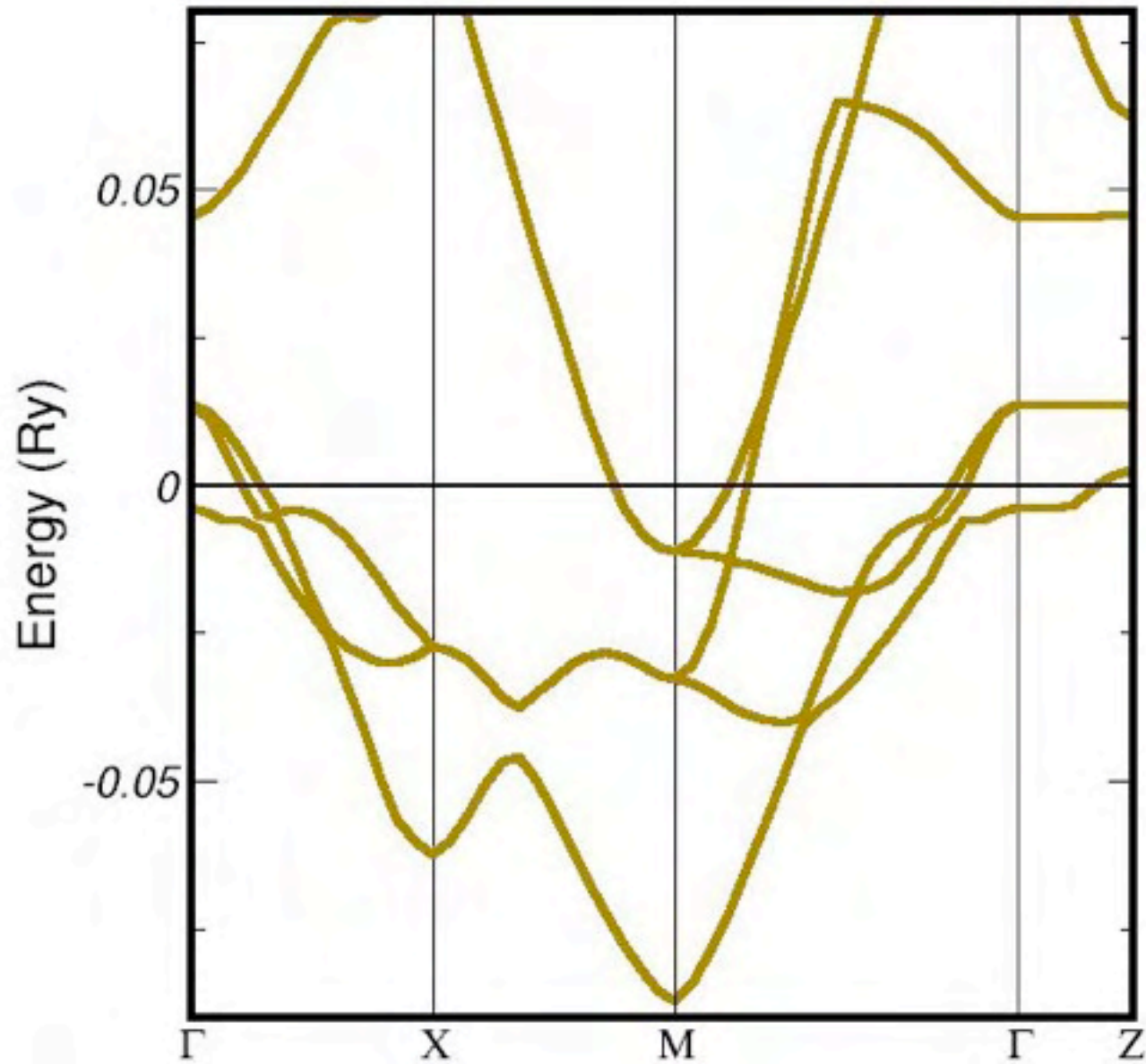
55K SmFeAsO<sub>0.9</sub>F<sub>0.1</sub>

56K Sr<sub>0.5</sub>Sm<sub>0.5</sub>FeAsF

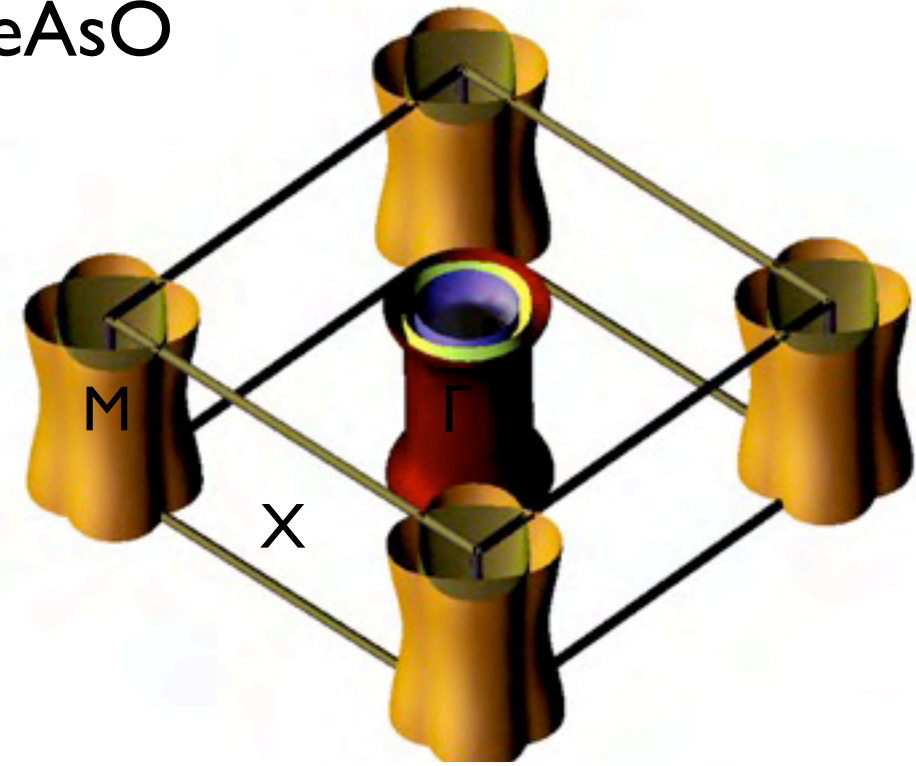
Superconductivity is achieved through:  
electron doping, hole doping, or pressure



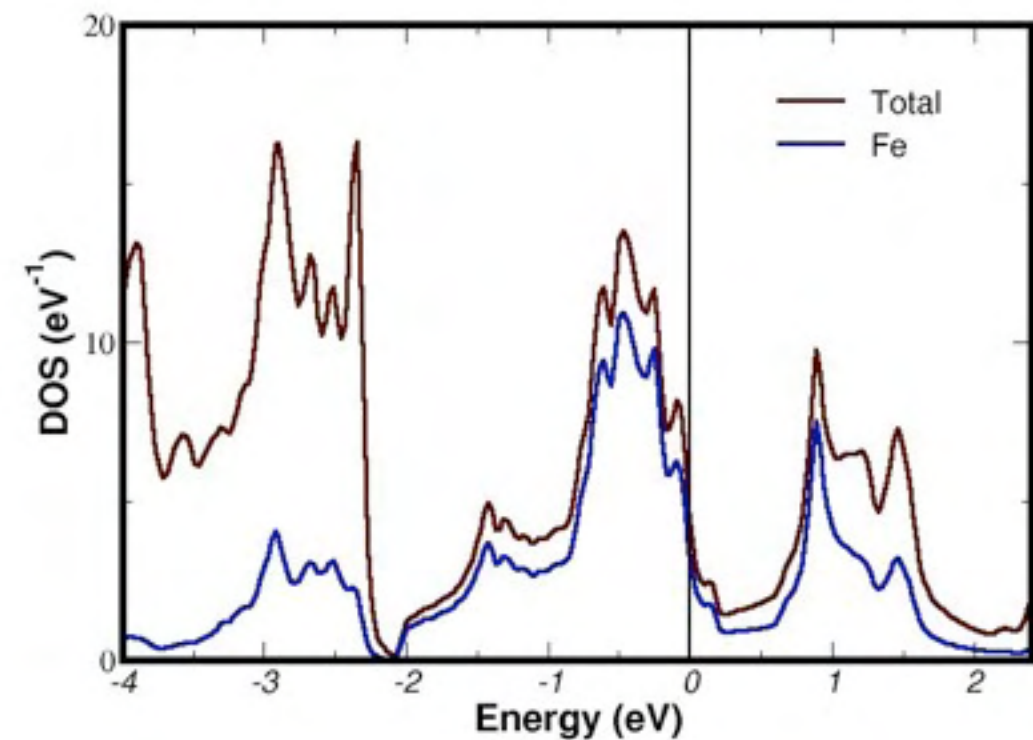
# Electronic structure



LaFeAsO



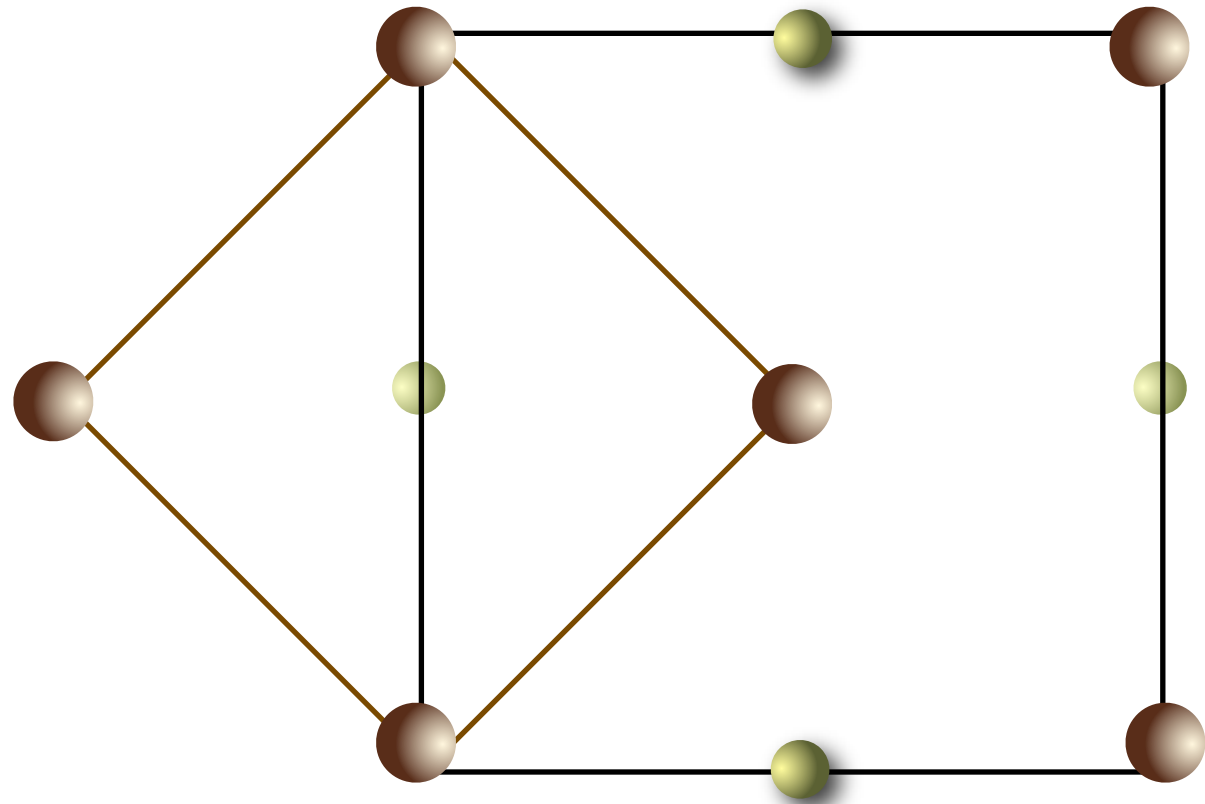
- Two columnar sets of FSs (1 hole, 1 e<sup>-</sup>)
- States at E<sub>F</sub> predominantly Fe *d*
- Pseudogap near E<sub>F</sub>
- Gap *not* t<sub>2g</sub>-e<sub>g</sub> derived



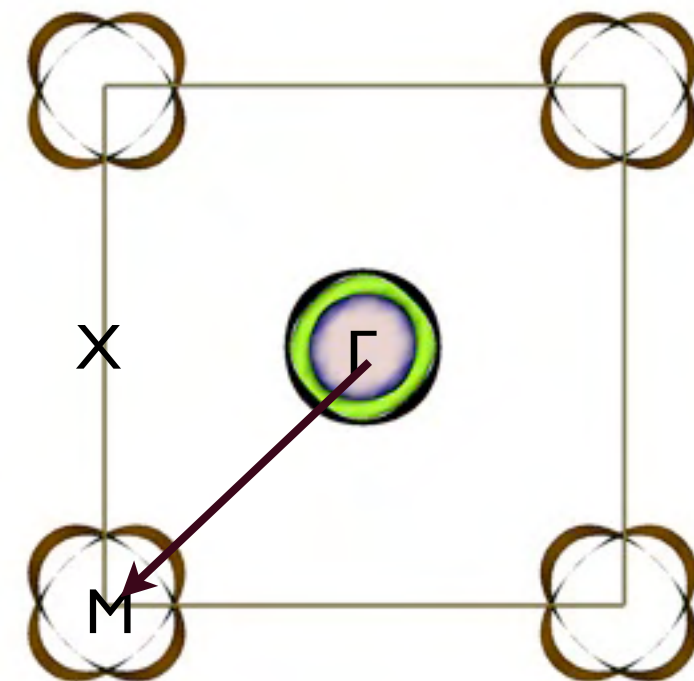
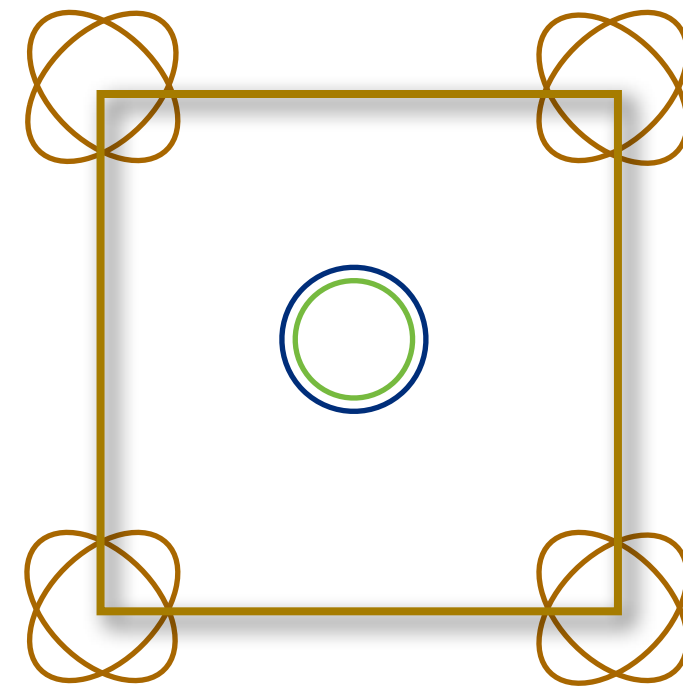




# Development of Fermi surface



Strong nesting tendencies along  $\Gamma$ -M

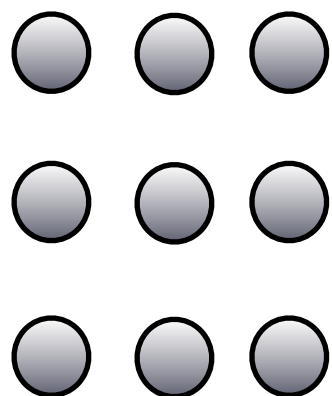




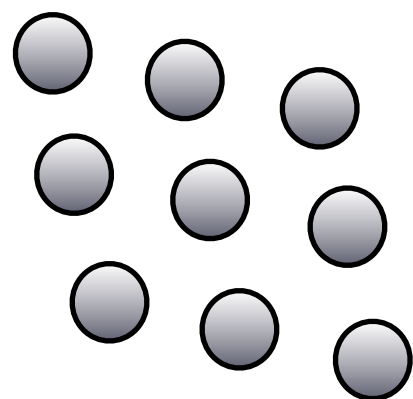
# Two phase transitions

## I) Structural Transition

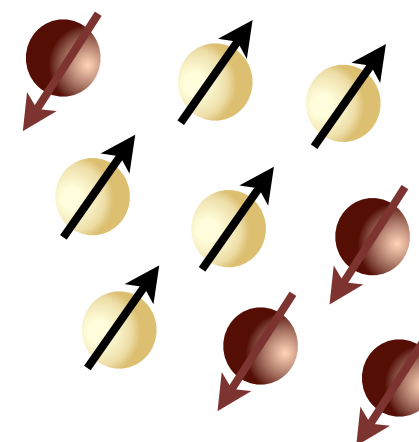
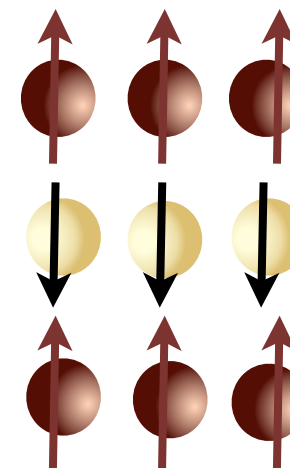
I22/IIII



FeTe



## II) Magnetic Transition



Transitions are simultaneous for FeTe and I22's, but structural transition is first in IIII's

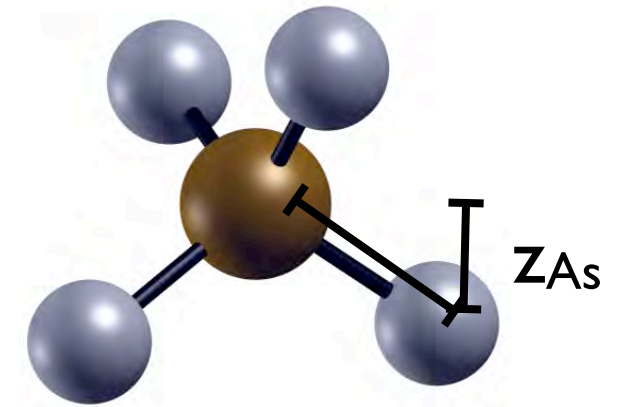
This is *opposite* of what calculations tell us



# Fe-based pnictides are almost always magnetic

- Relaxation of non-magnetic system (even in GGA) results in a vastly underestimated Fe-As distance

	non-magnetic	spin-polarized	experiment
Fe-As	2.32 Å	2.41 Å	2.40 Å
As	1.97 Å	1.99 Å	1.98 Å
$Z_{As}$	1.22 Å	1.35 Å	1.36 Å

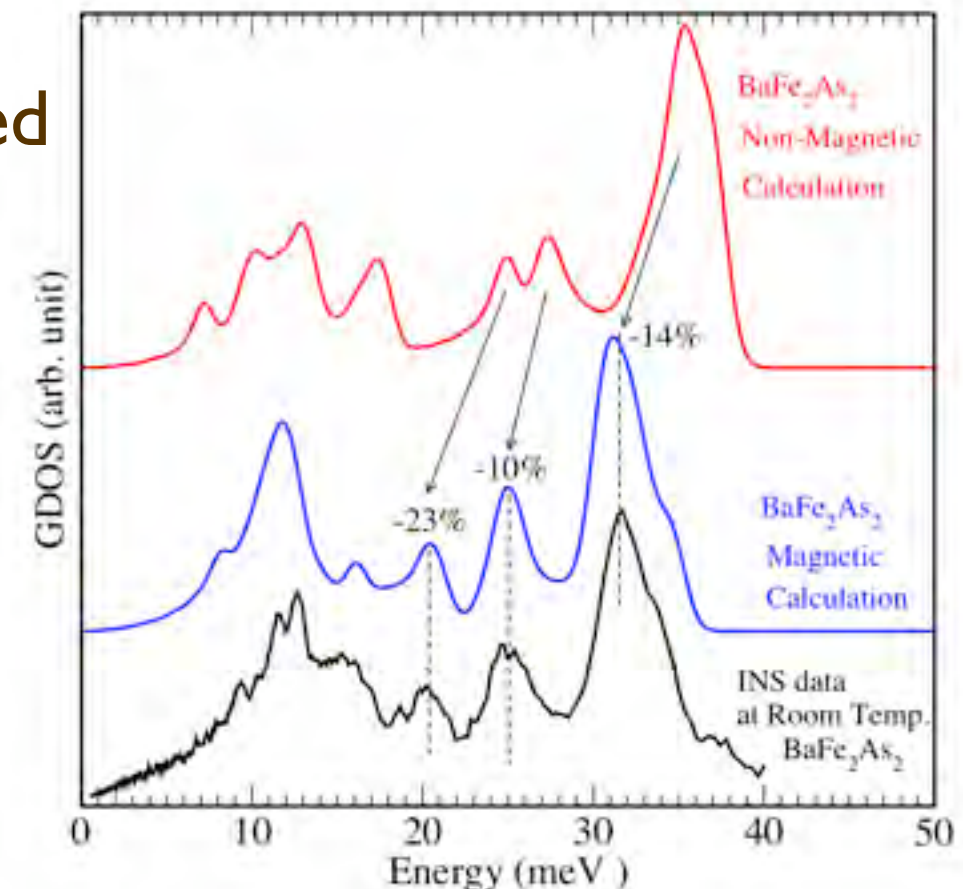


Z.P.Yin et al. PRL **101**, 047001 (2008)

Spin-polarized relaxation is correct to within .8%

- Non-magnetic phonon spectrum is strongly shifted from experiment

Spin-polarized spectrum is vastly improved

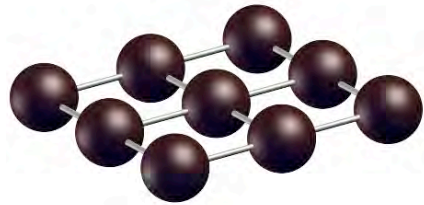


T.Yildirim arXiv: 0902.3462

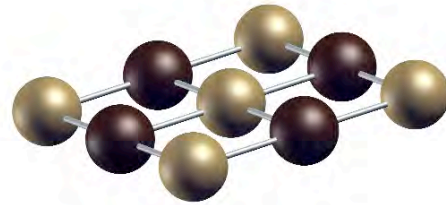


## Fe-based pnictides are magnetic *above* $T_N$

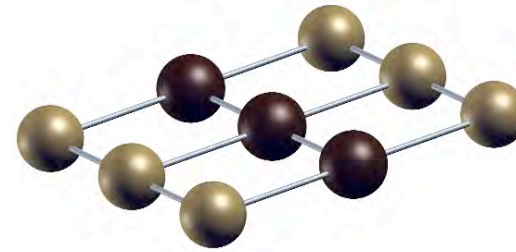
- Structural distortion not reproduced in non-magnetic case (or *wrong* magnetic case)



Non-magnetic



Checkerboard



Stripe

Spin-polarized calculations reproduce (predict!) distortion to within .6% of observed values

Calculations indicate that magnetism is a condition for distortion, not a result of distortion

Conclusion: compounds are magnetic locally, though not ordered, even above the structural transition temperature





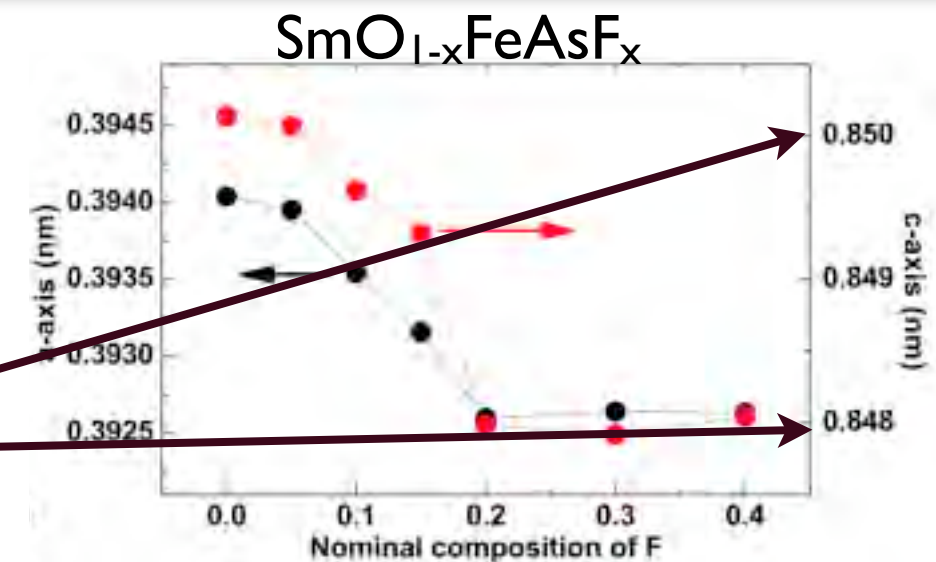
# Superconducting Fe-based pnictides are magnetic below

Fe-As distance “constant” as a function of doping

A dramatic contraction would occur if Fe became non-magnetic

$$\Delta c\text{-axis} = 2\Delta z_{\text{As}} = .026 \text{ nm}$$

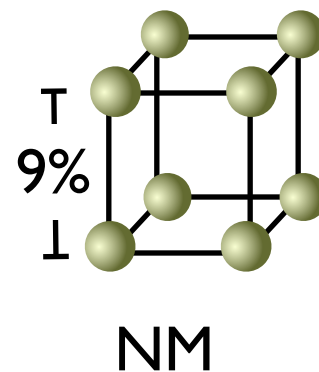
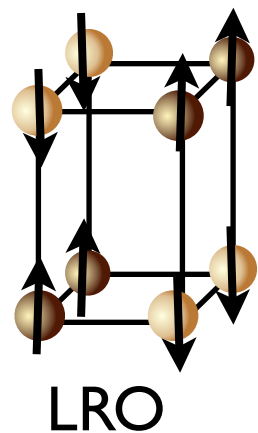
(.002 nm)



Liu *et al.* PRL **101**, 087001 (2008)

Where magnetism has definitively been killed, so has superconductivity

CaFe<sub>2</sub>As<sub>2</sub>: Orthorhombic → Collapsed Tetragonal



W.Yu *et al.* PRB **79**.020511 (2009)

Long range magnetic order is detrimental to superconductivity

Spin fluctuations provide the pairing mechanism





# Magnetism is the key

To understand these systems, we must understand the magnetism.

- How does magnetic state arise?
- How is it suppressed by doping?
- How is it suppressed by pressure?

Nature of the magnetic interaction

- i) Superexchange
- ii) Nesting-driven itinerant magnetism

(neither!)



# Methodology

## GGA

Best for structural optimization, but magnetism vastly overestimated

$$\mu_B = 2.1 \text{ (vs. 0.9 in exp. for 122)}$$

## LDA

Less magnetic than GGA, but less accurate for structural properties

$$\mu_B = 1.6$$

For comparison with experiment (e.g. quantum oscillations), we apply a negative  $U$  within the LDA+ $U$  formalism

- Achieve experimental moment by tuning  $U$
- With  $U$  large enough to suppress moment fully, FS is very close to non-magnetic one

## Codes

Wien2K

VASP

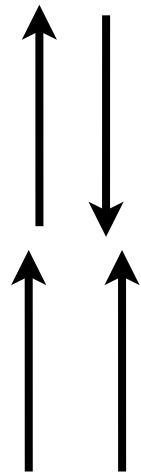


# Spin fluctuations as a pairing mechanism

$$\Delta_{k\alpha} \sim \sum_{q\beta} V_{kq\alpha\beta} \Delta_{q\beta}$$

$\Delta_{k\alpha}$  = gap at  $k$ , on surface  $\alpha$

$V_{kq\alpha\beta}$  = pairing between surfaces  $\alpha, \beta$  at respectively,  $k, q$



For singlet pairing,  $V$  is always negative (repulsive)

For triplet pairing,  $V$  is always positive





# Spin fluctuations as a pairing mechanism

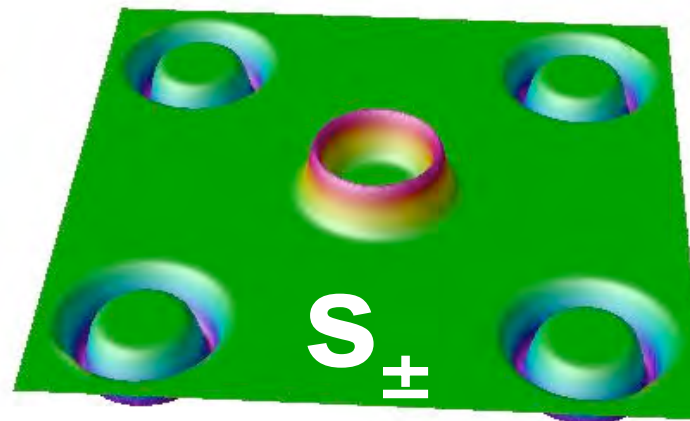
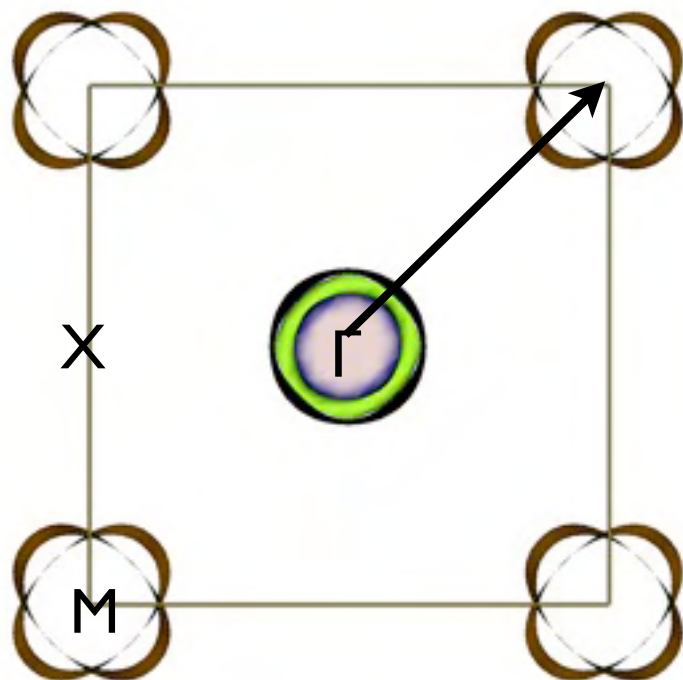
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$$\Delta_{k\alpha} \sim \sum_{q\beta} - \Delta_{q\beta}$$

Gaps on surfaces connected by SF must have opposite signs



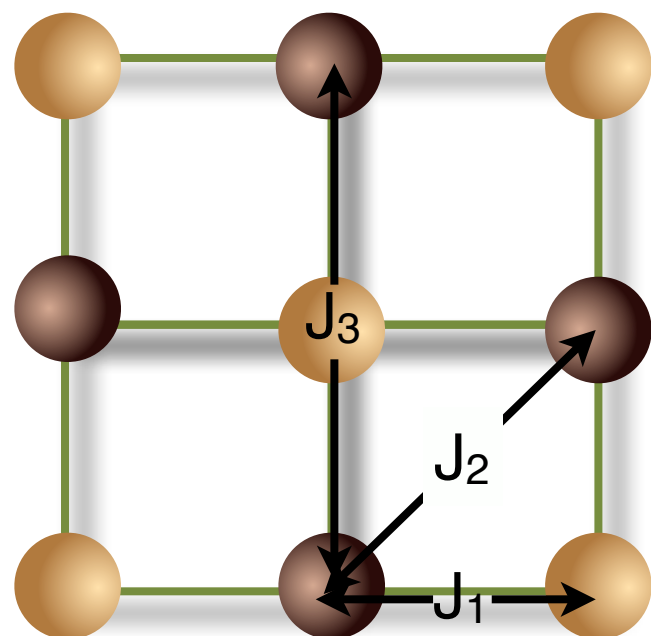
S<sub>+/-</sub>

- Pairing provided by nesting-driven SF
- Full gap on both surfaces with phase shift between them



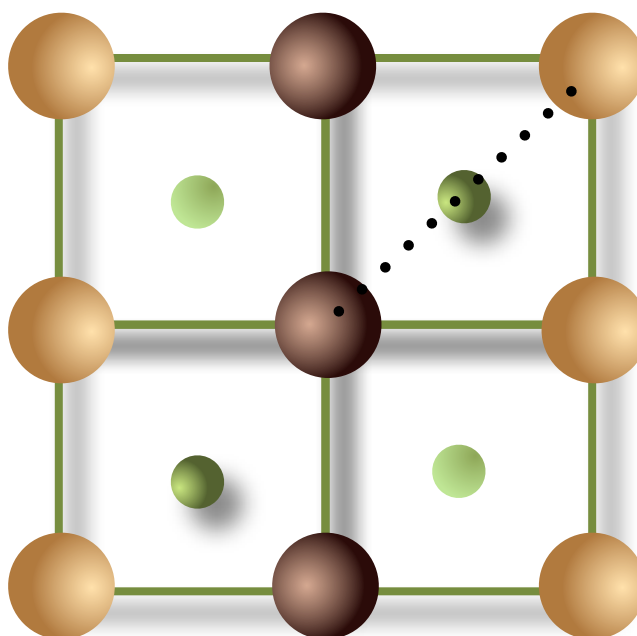
# Energetics in the superexchange picture

## Checkerboard



$$\Delta E = 2J_1 - 2J_2 - 2J_3$$

## Stripe (SDW)

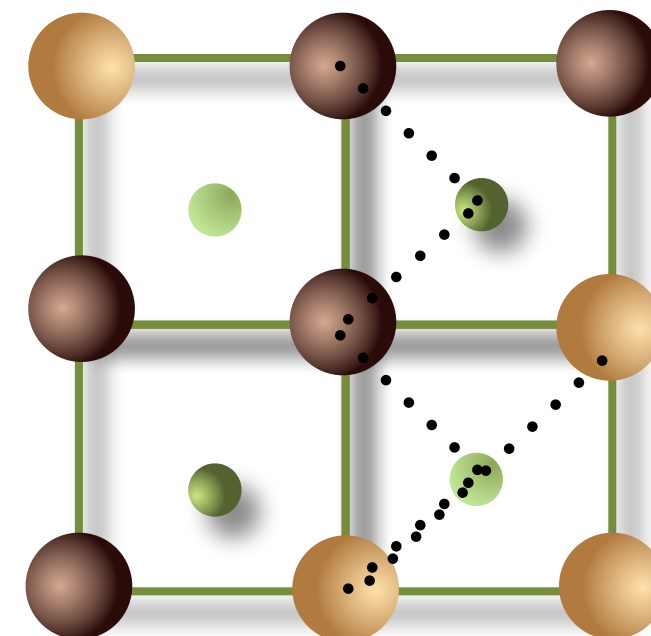


$$\Delta E = 2J_2 - 2J_3$$

\* (1111, 122)

$$J_2 > J_1/2$$

## Doublestripe



$$\Delta E = 2J_3$$

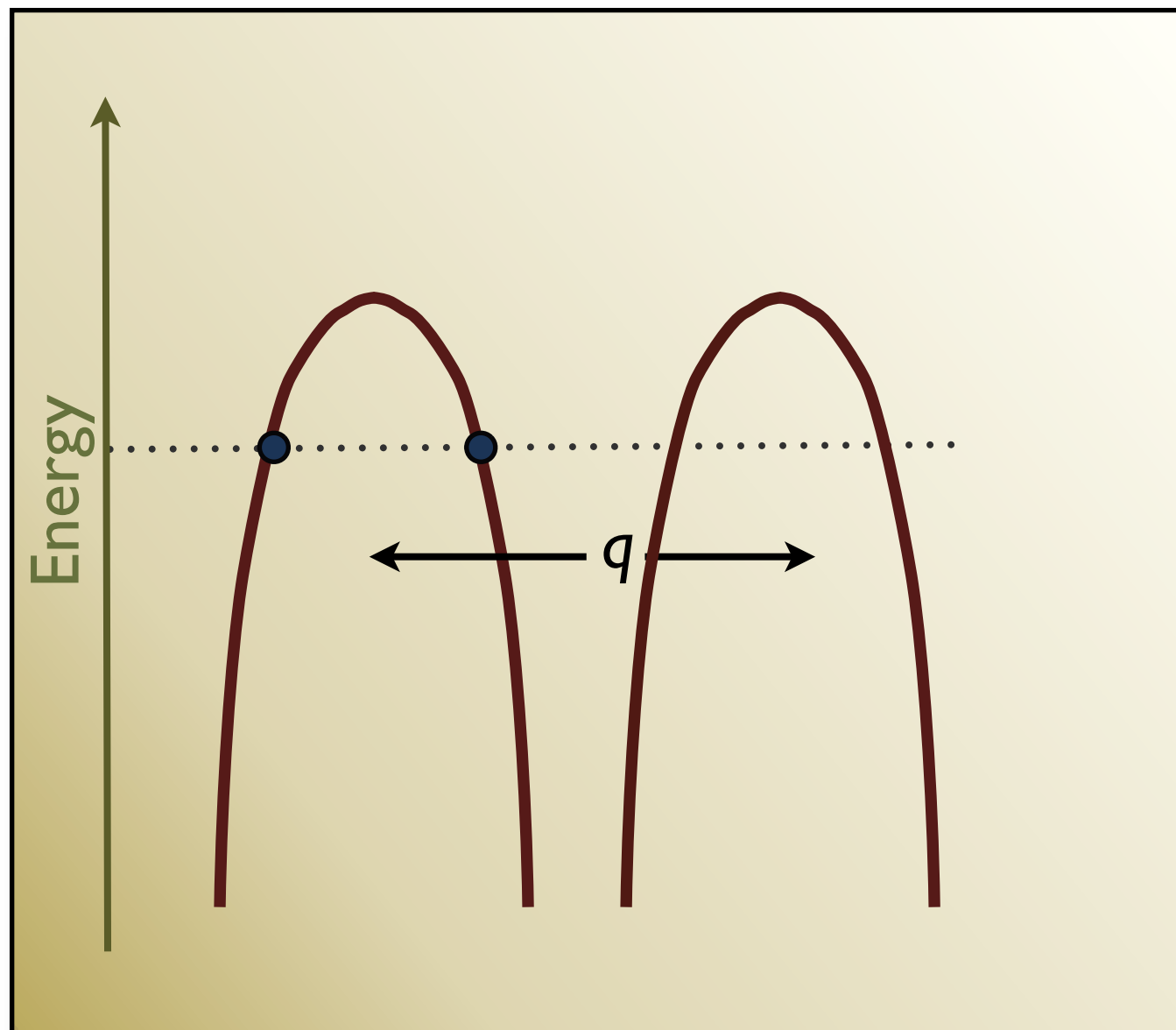
\* (FeTe)

$$J_3 > J_2/2$$

Superexchange is an untenable mechanism for double stripe order



# Are nesting and magnetism related?



## Nesting function

$$\chi''(q, \omega) / \omega = \sum_k \delta(\epsilon_F) \delta(\epsilon_k - \epsilon_{k+q})$$

$\omega \rightarrow 0$

Only Fermi surface points contribute

## Real part of susceptibility

$$\chi'(q, 0) = \sum_k \frac{f(\epsilon_k) - f(\epsilon_{k+q})}{\epsilon_k - \epsilon_{k+q}}$$

Gathers from above and below  $E_F$

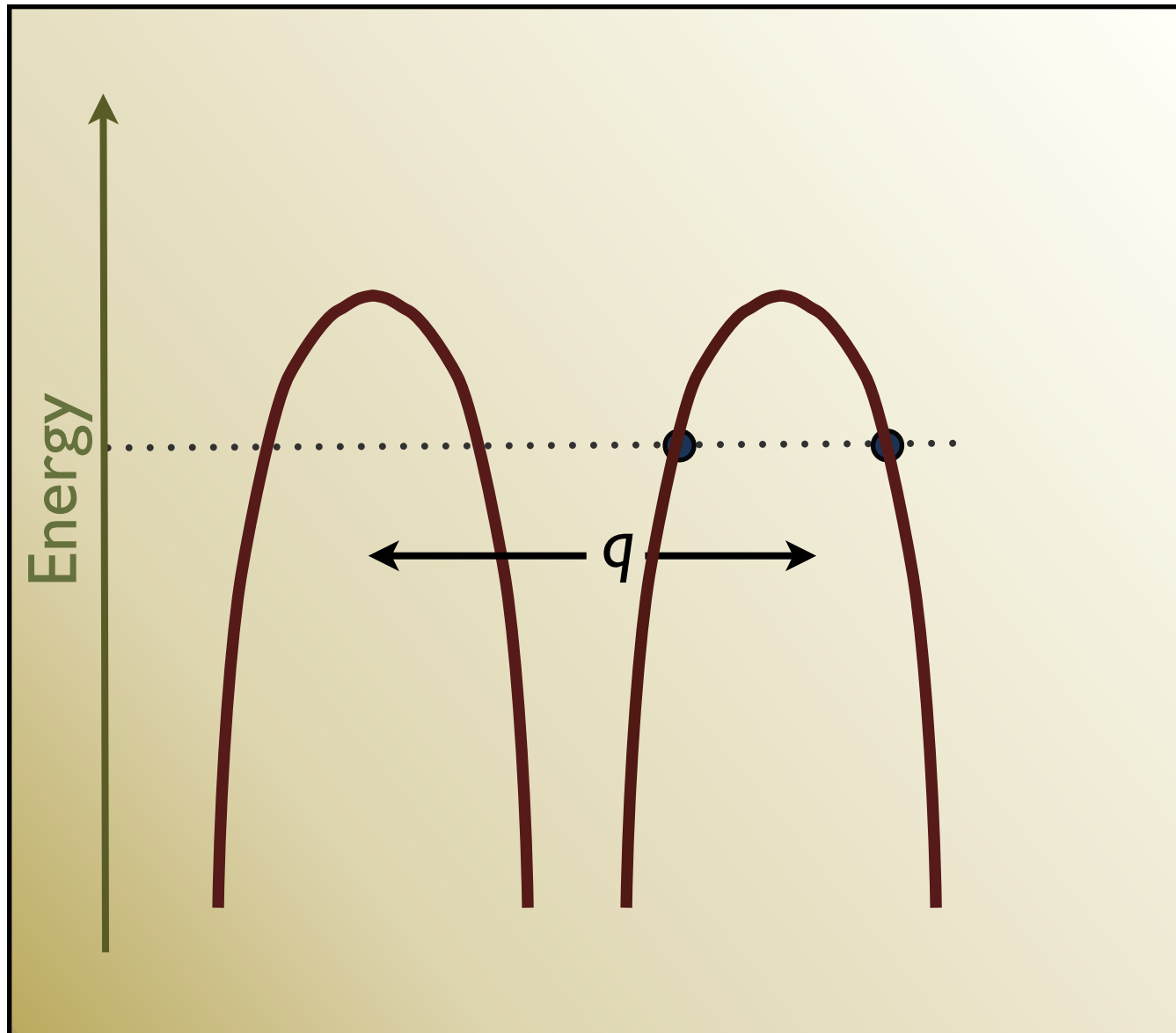
Nesting function can have a maximum at a different (sometimes very different) place in q-space than real part of  $\chi$

The *real part* is responsible for magnetic instability





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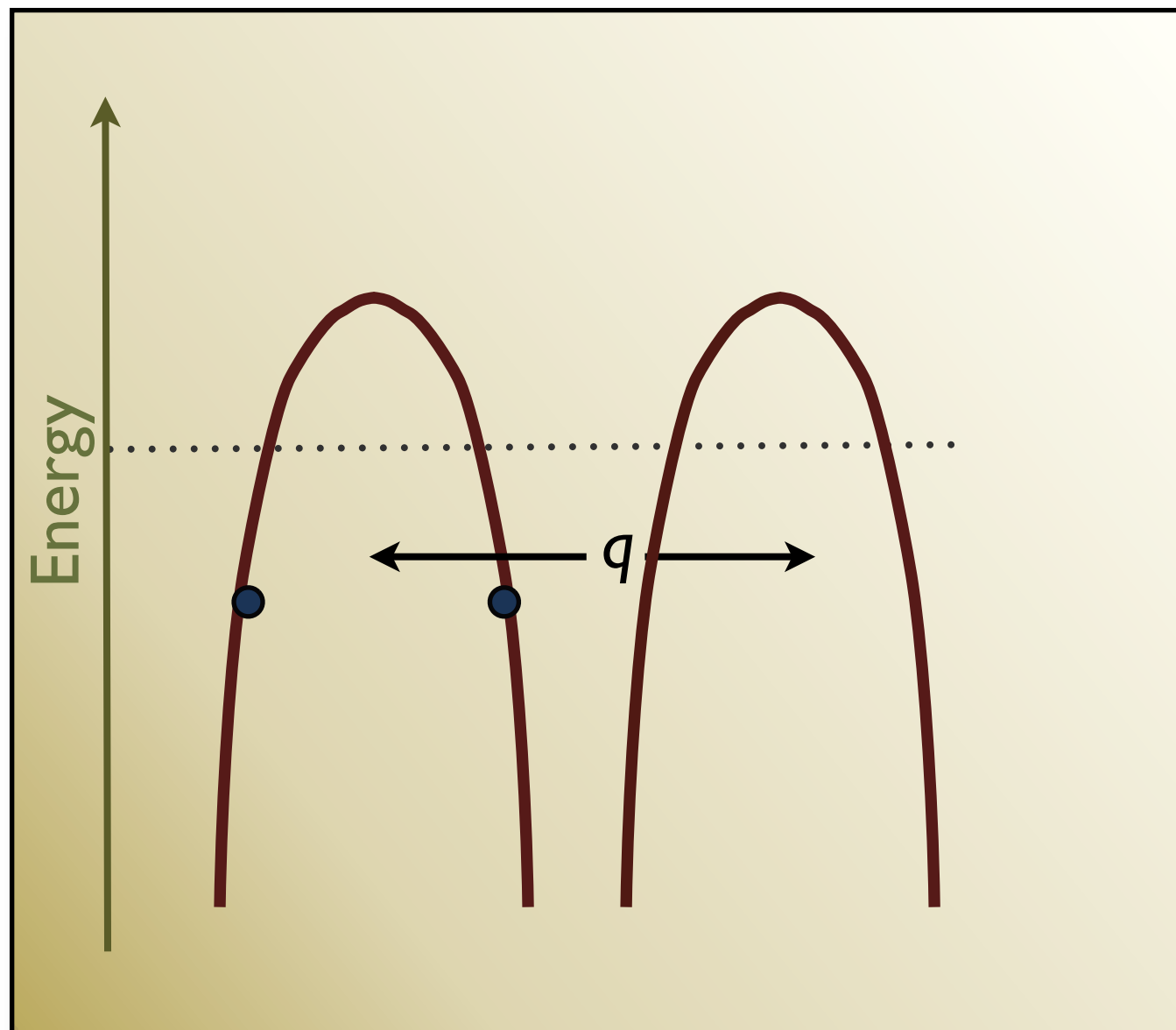
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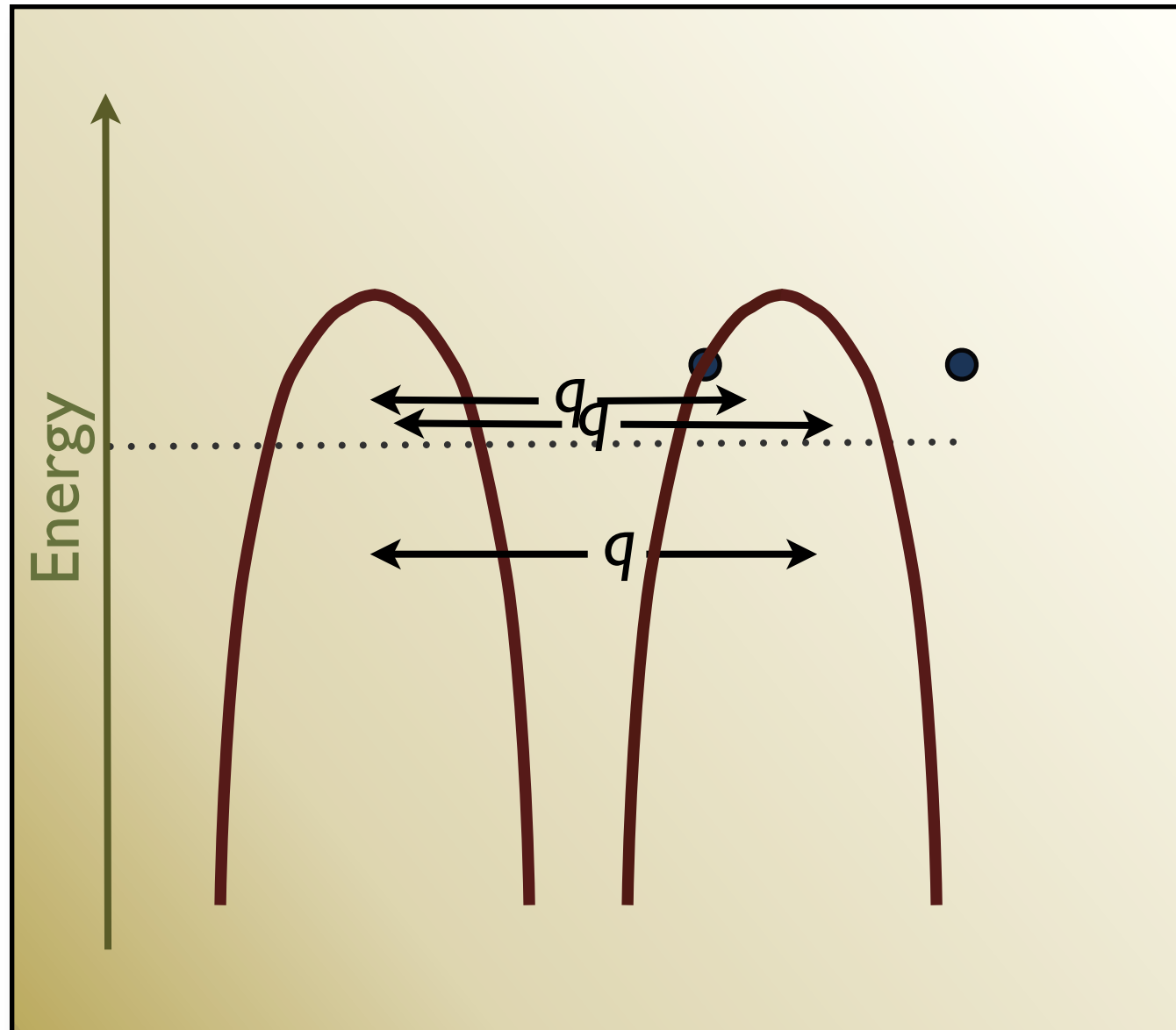
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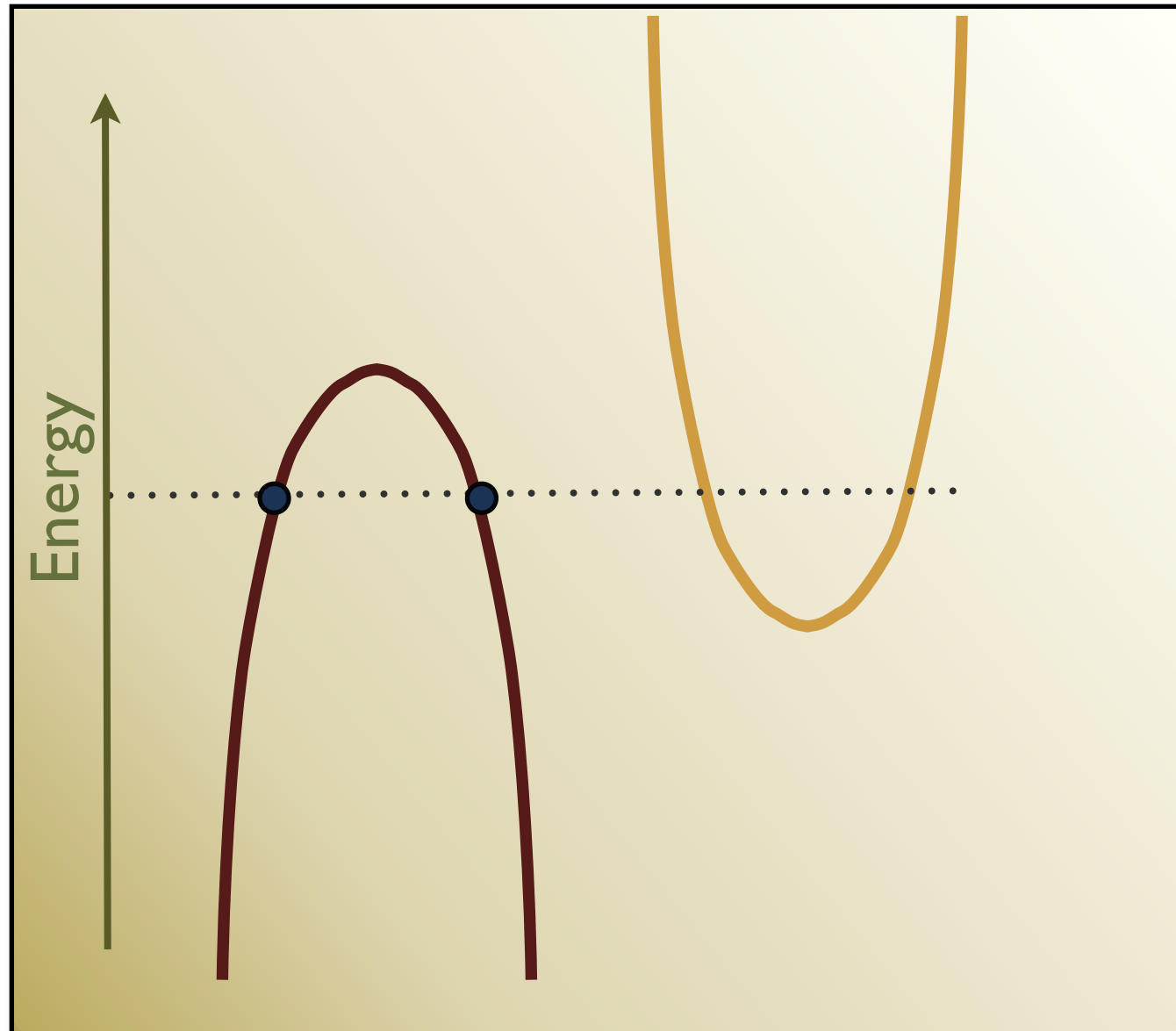
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# How does doping change nesting/magnetic properties?



Nesting function  
(Spin fluctuations)

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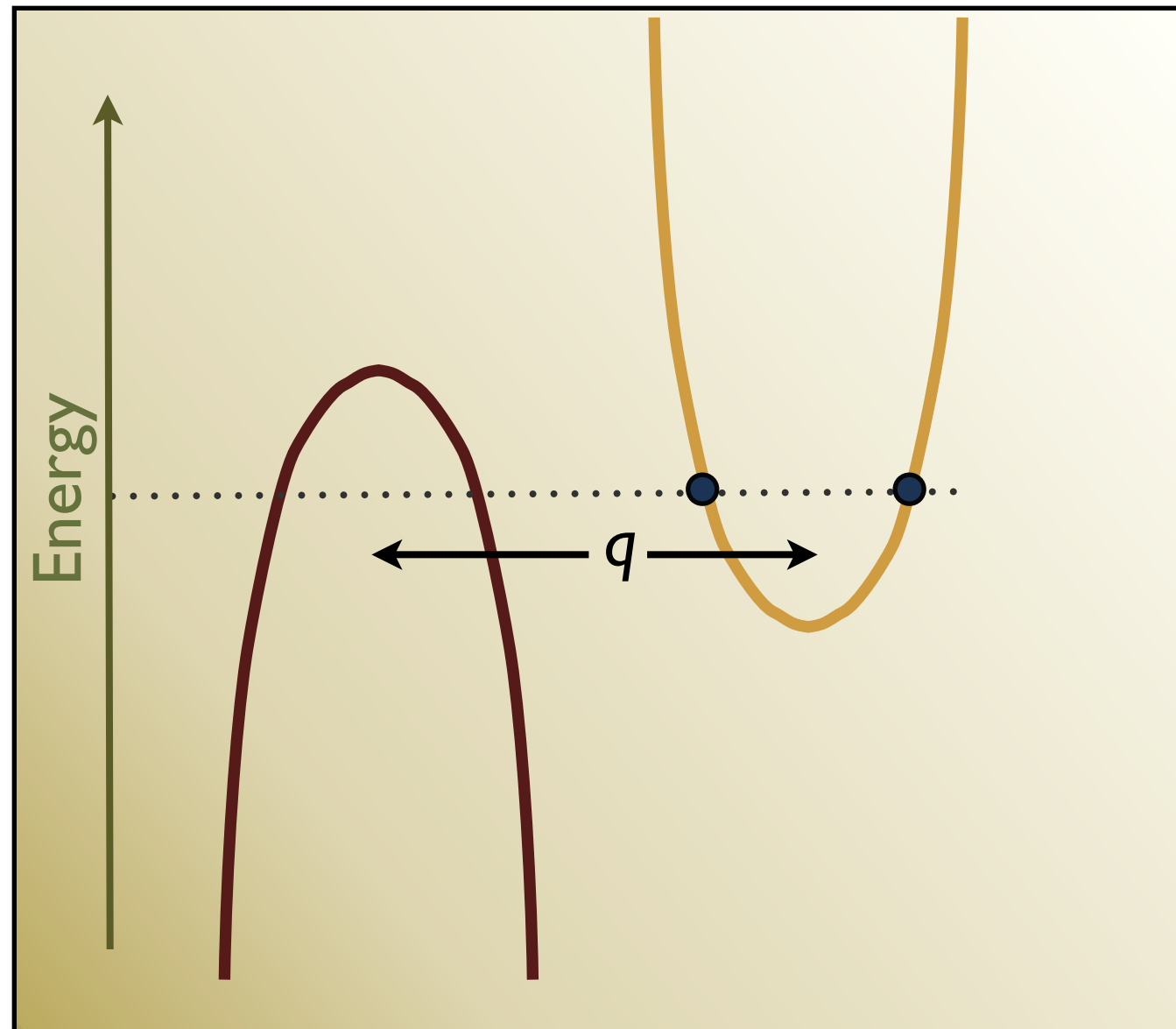
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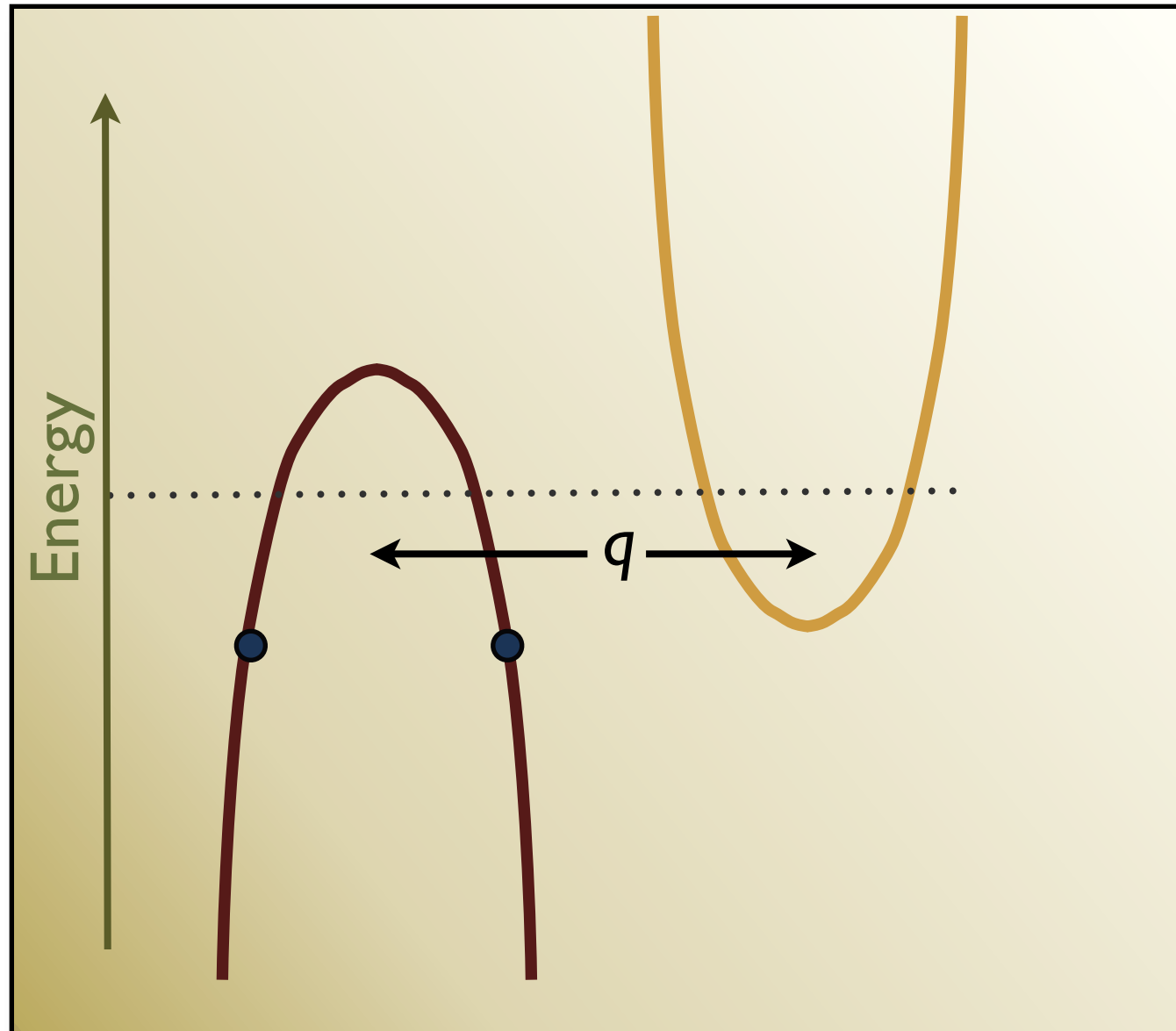
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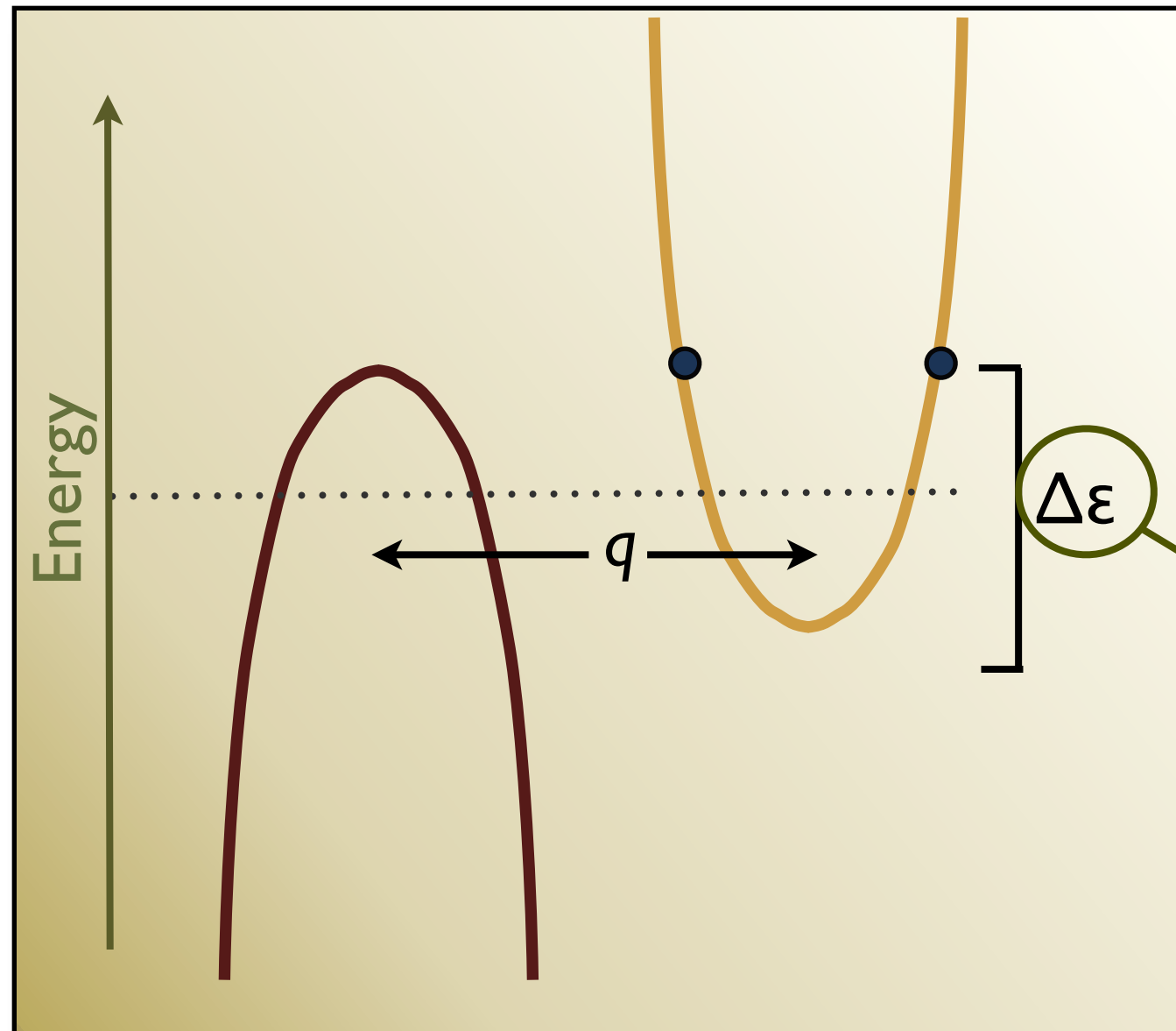
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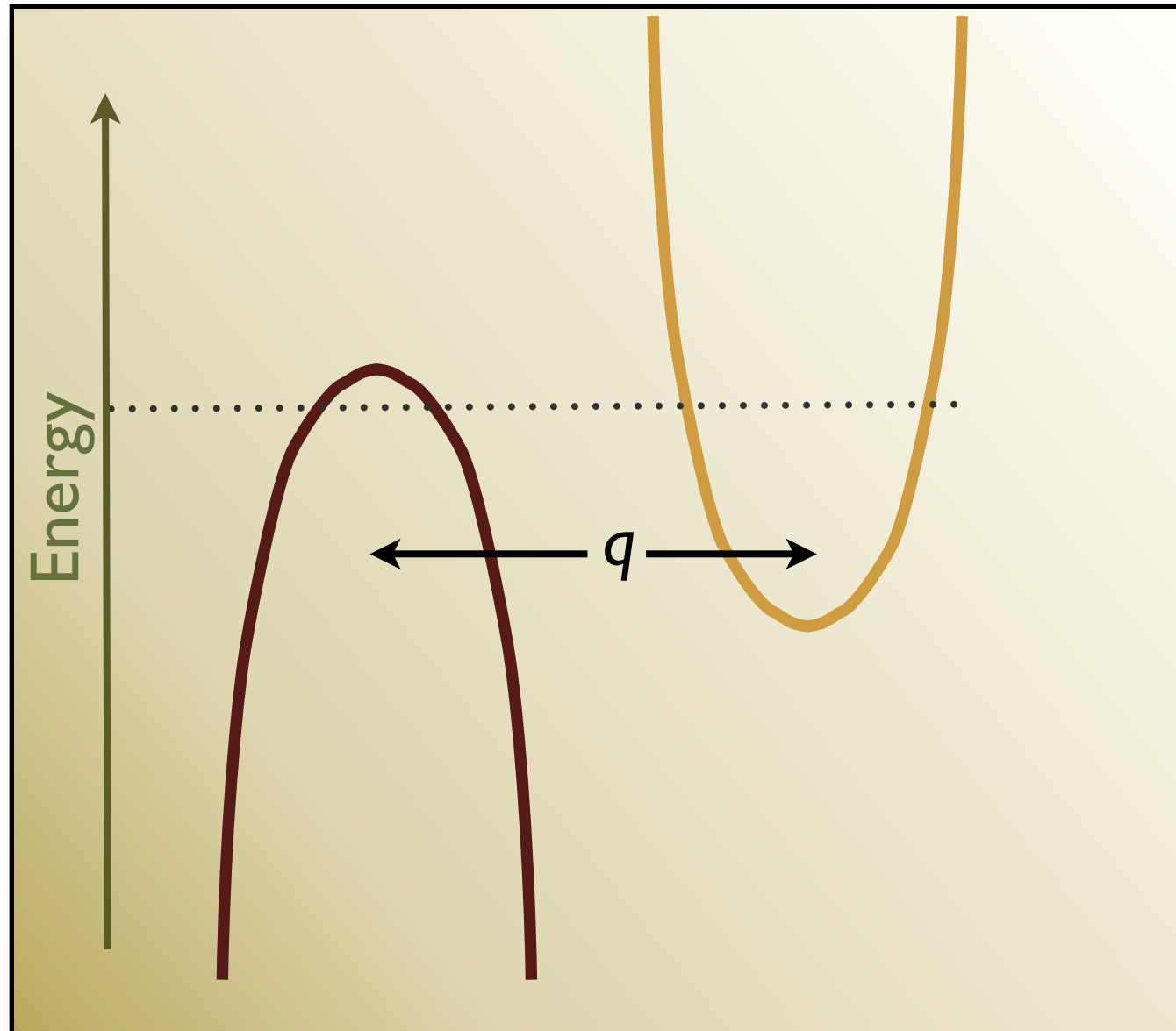
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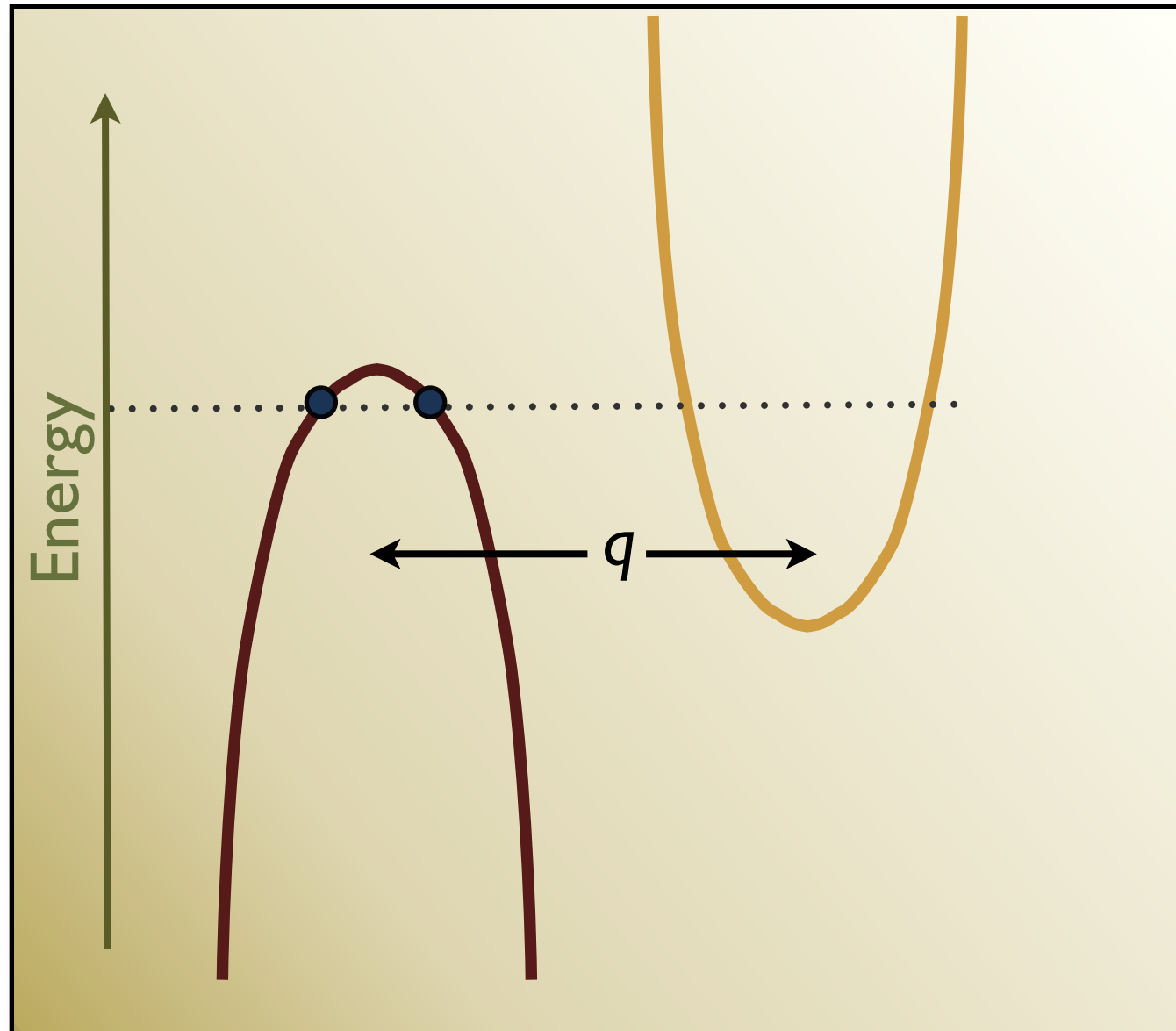
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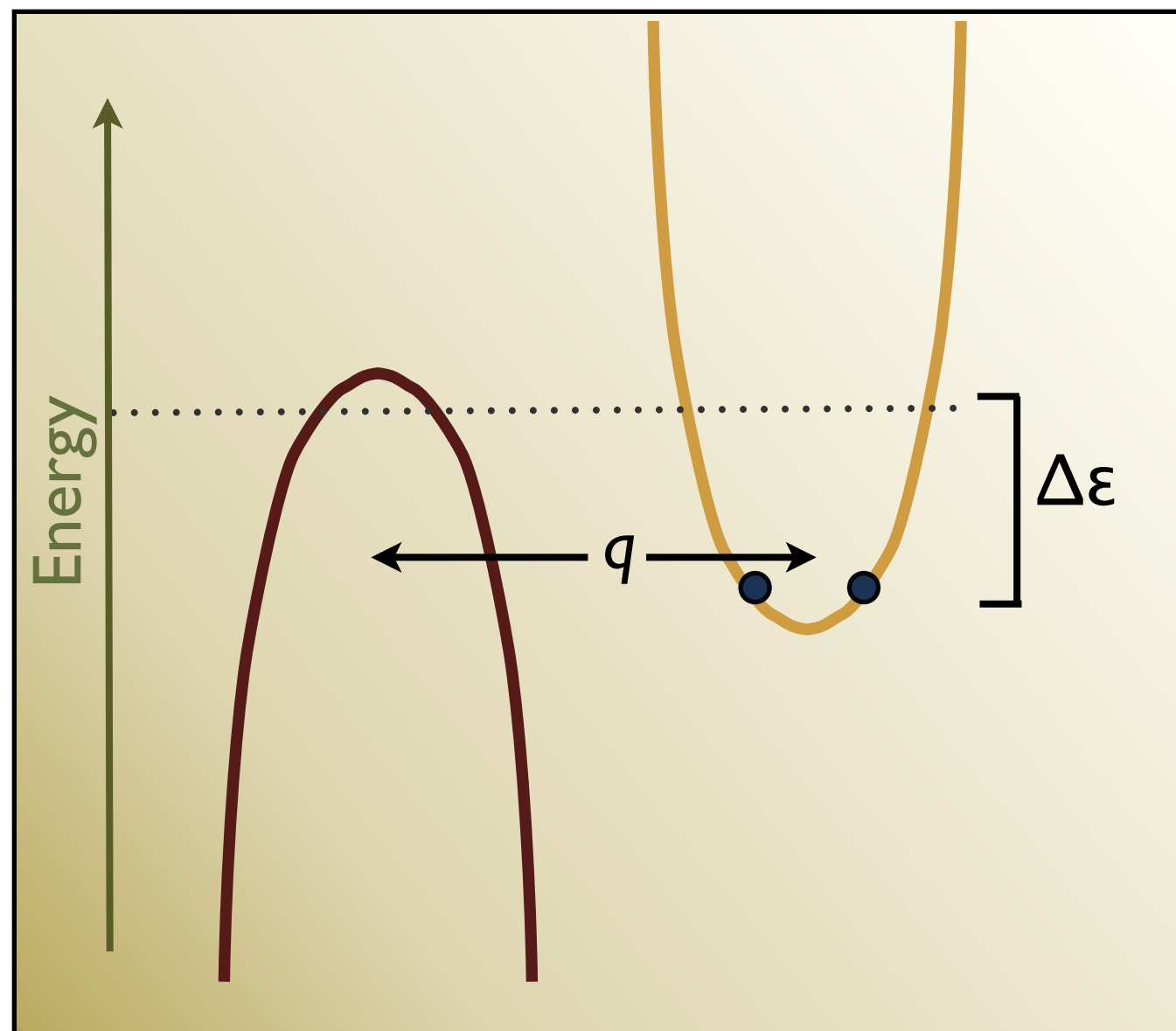
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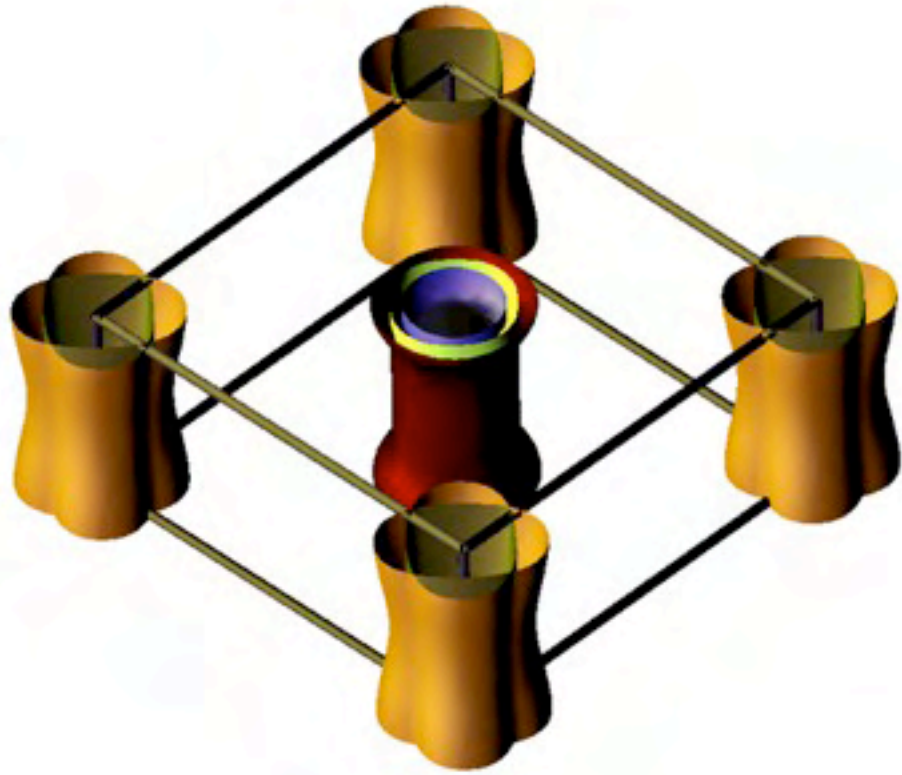
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Doping can 'select' between competitive phenomena

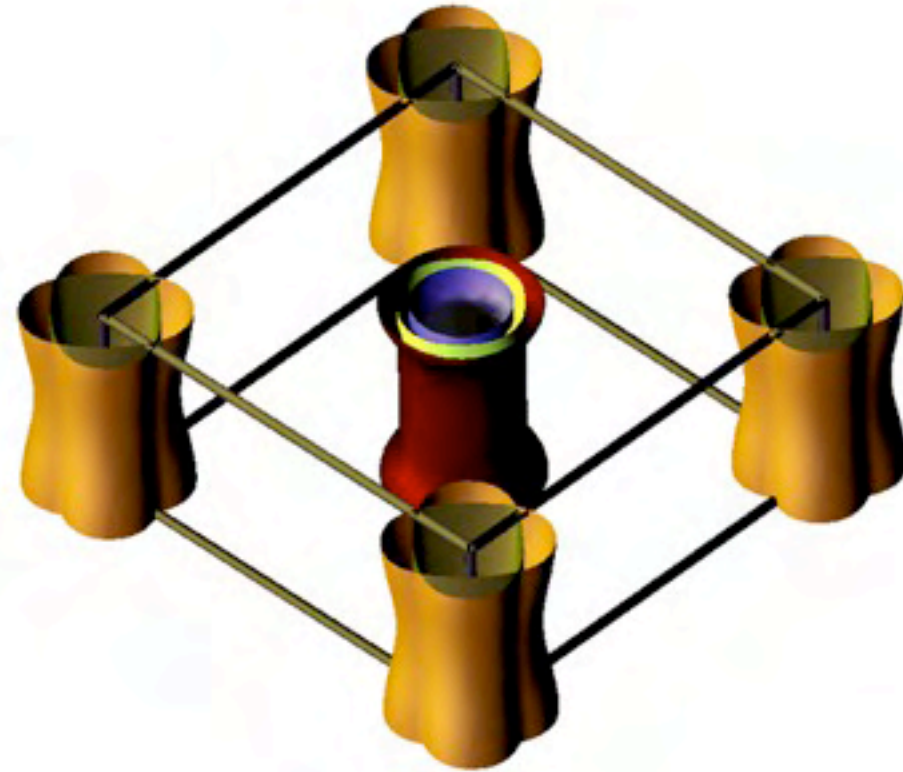




# Doping in the $1111$ systems



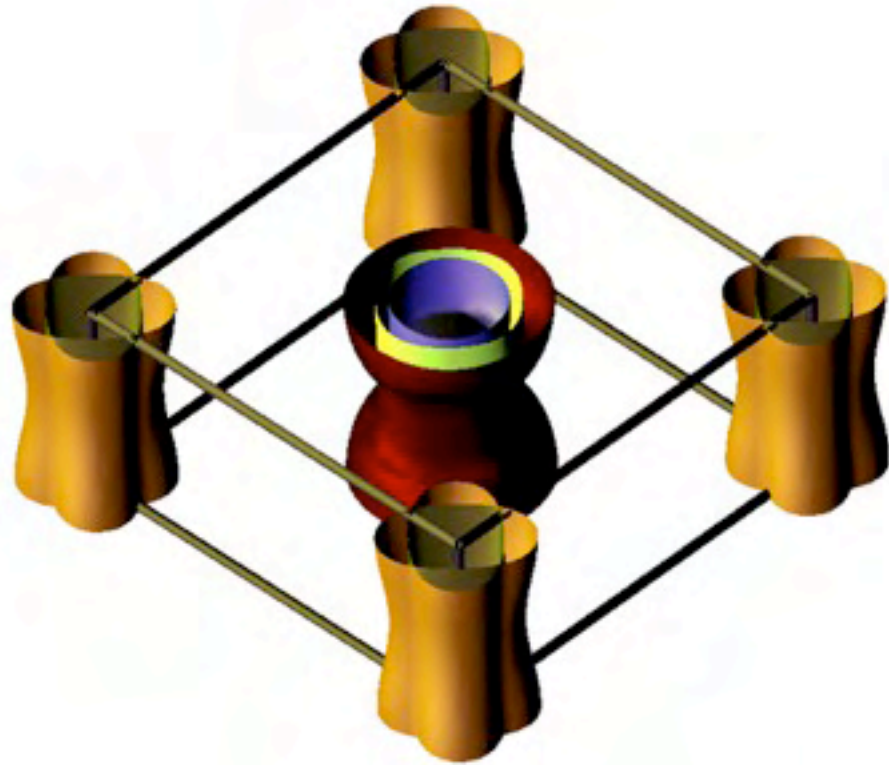
Hole doping



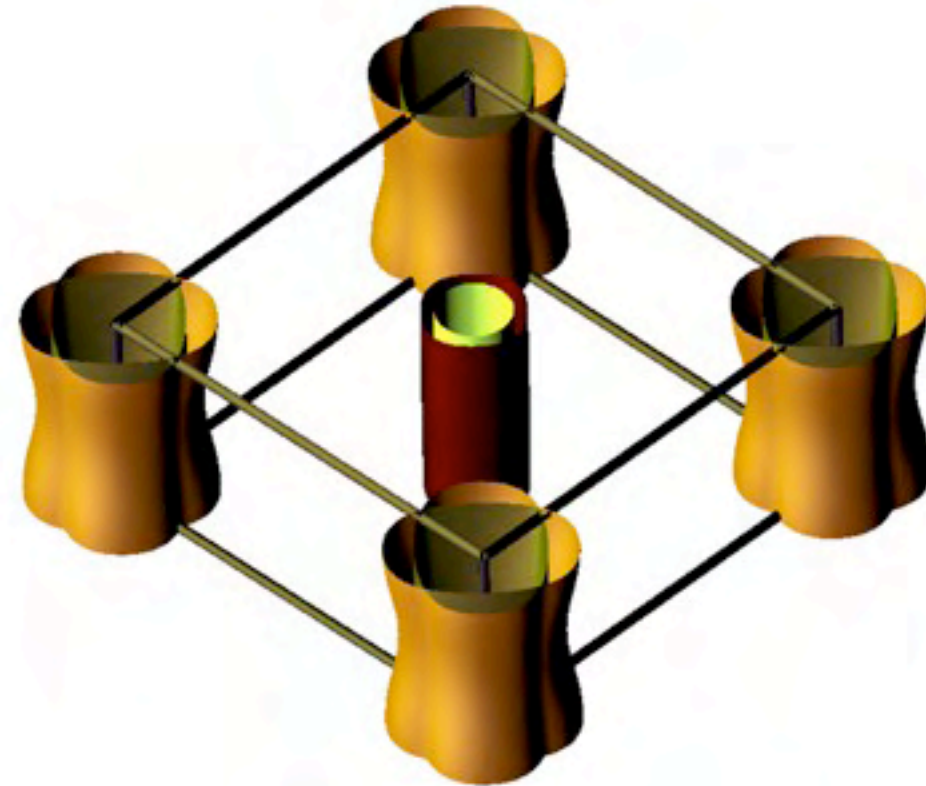
Electron doping



# Doping in the $1111$ systems



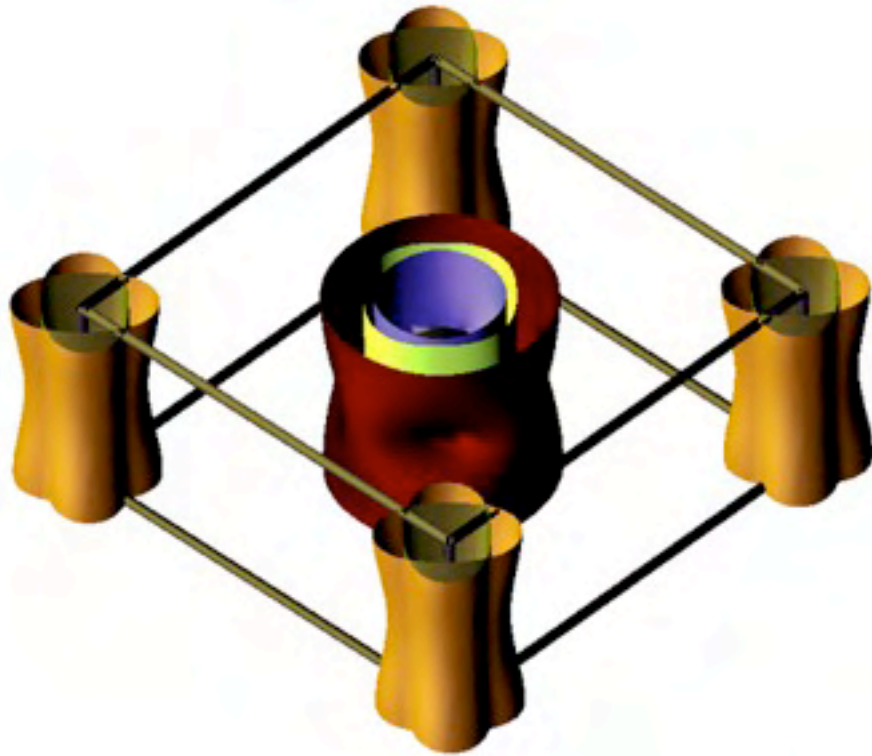
Hole doping



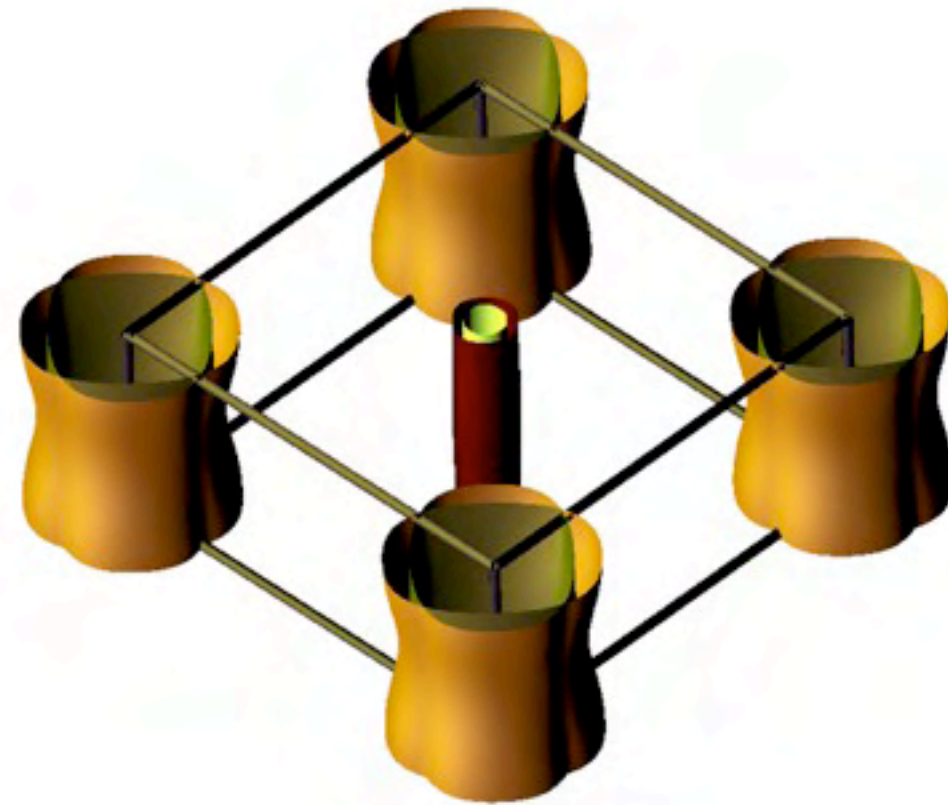
Electron doping



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Hole doping

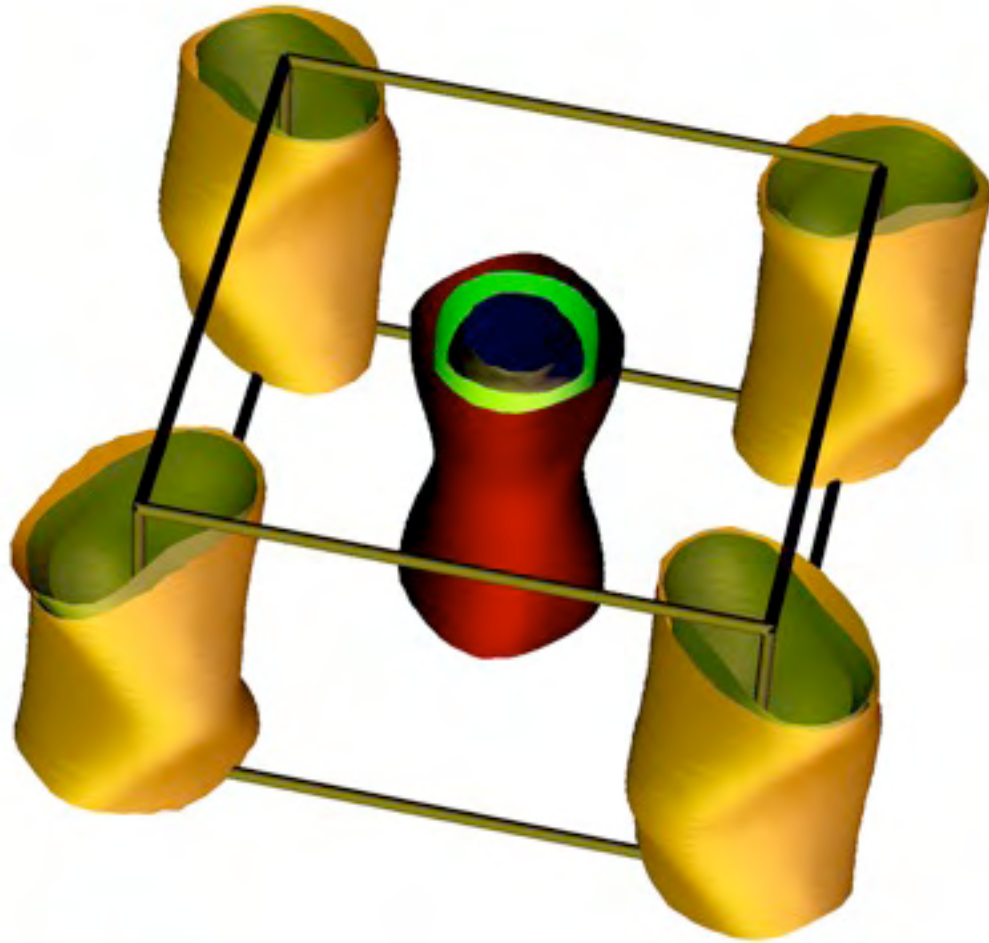


Electron doping

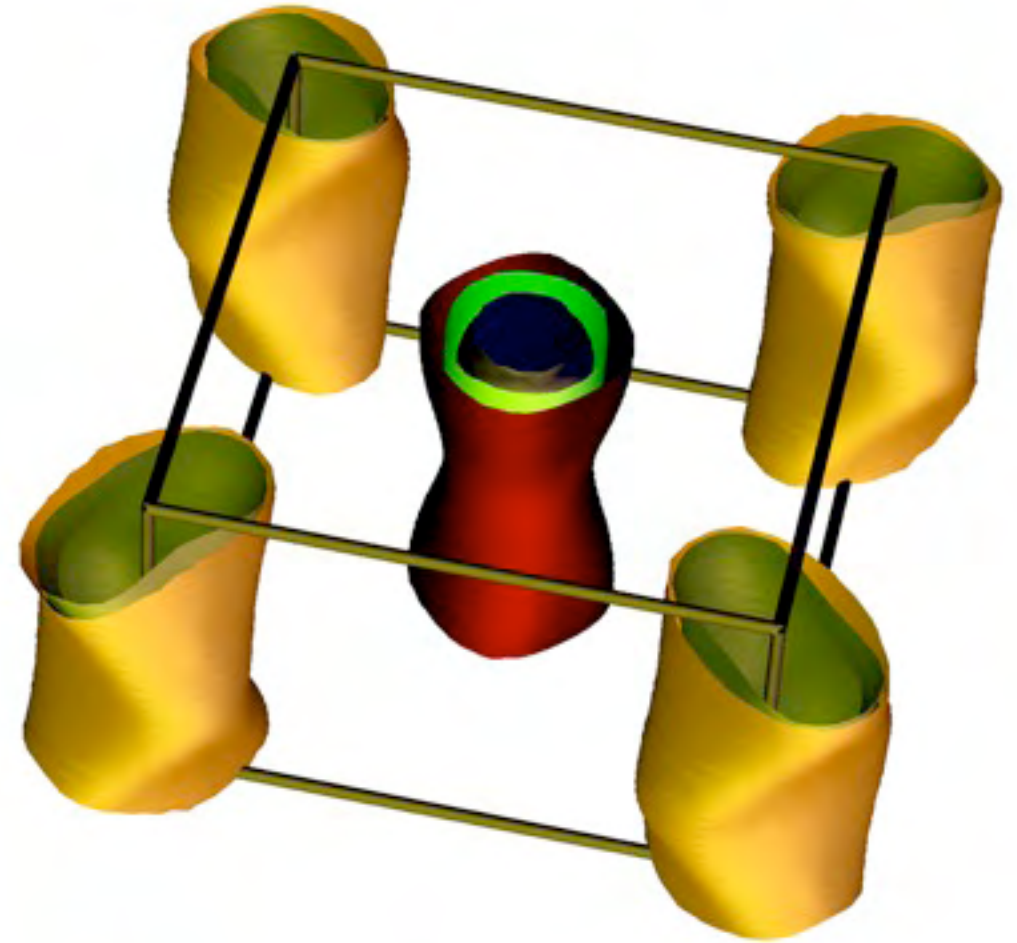




# Doping in the 122 systems



Hole doping  
 $\text{Ba}_{1-x}\text{K}_x\text{Fe}_2\text{As}_2$

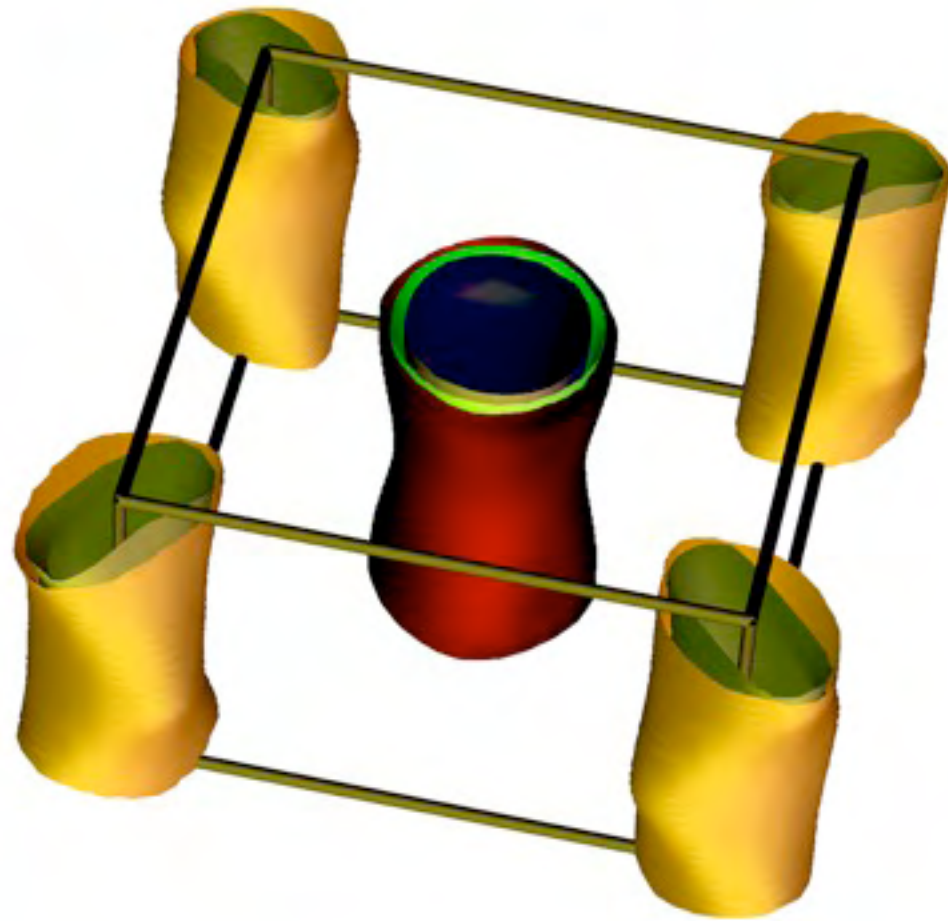


Electron doping  
 $\text{BaFe}_{2-x}\text{Co}_x\text{As}_2$

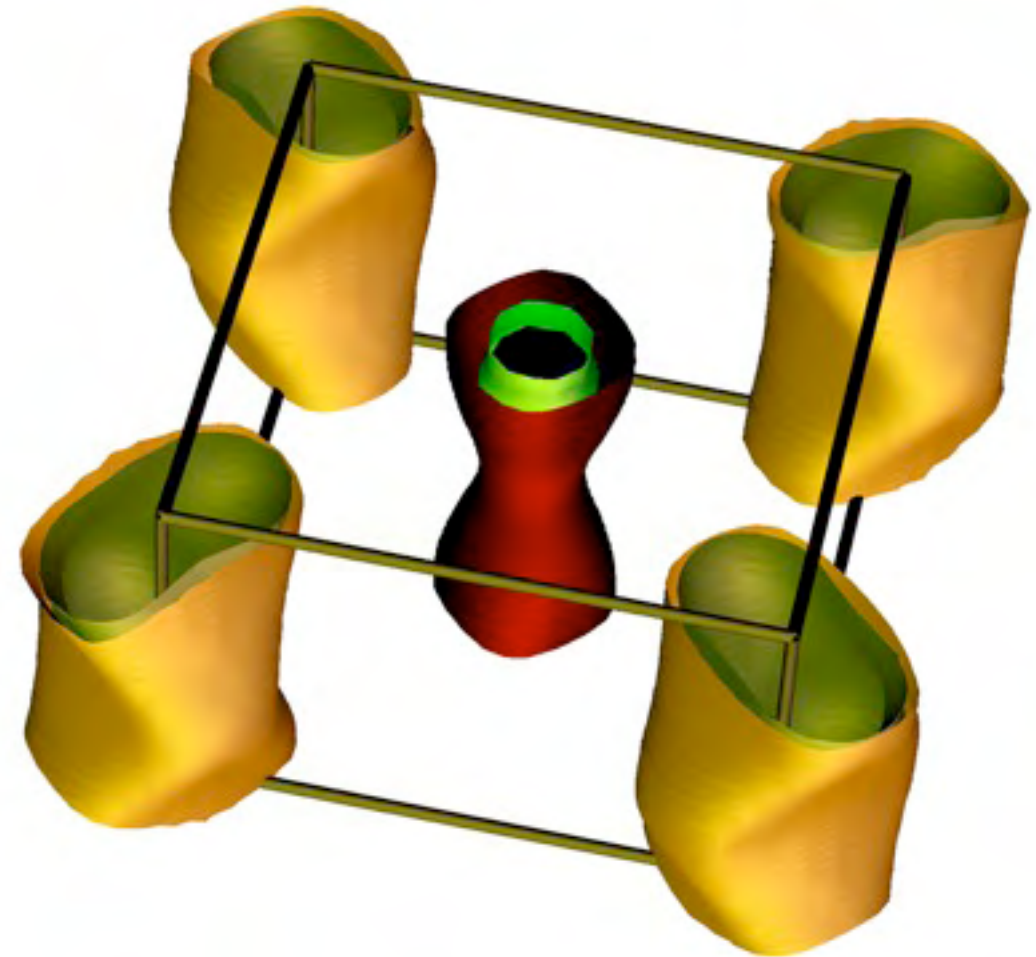




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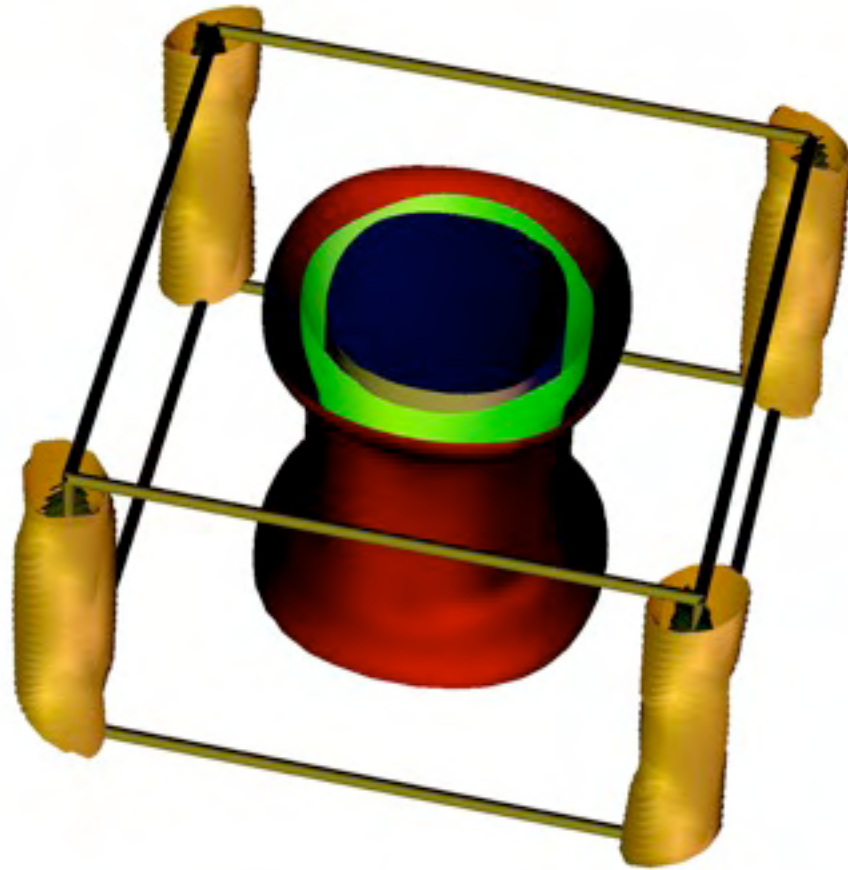
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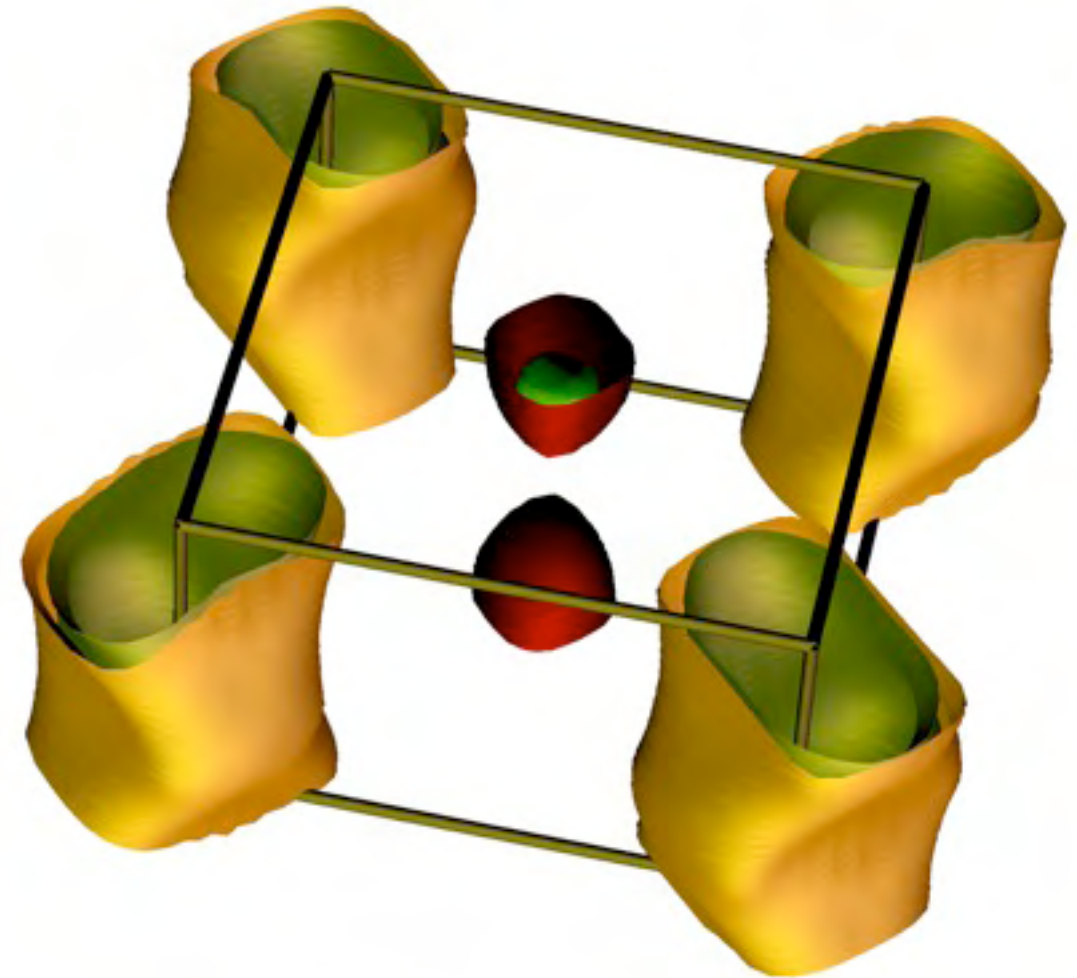
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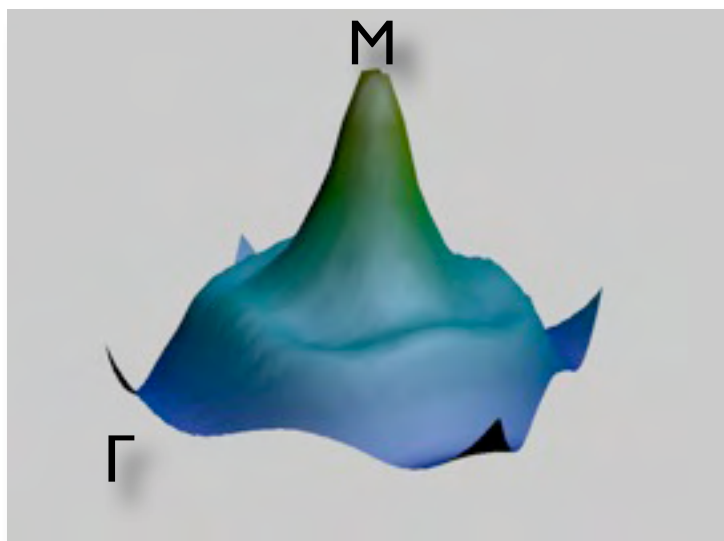


Electron doping  
 $\text{BaFe}_{2-x}\text{Co}_x\text{As}_2$

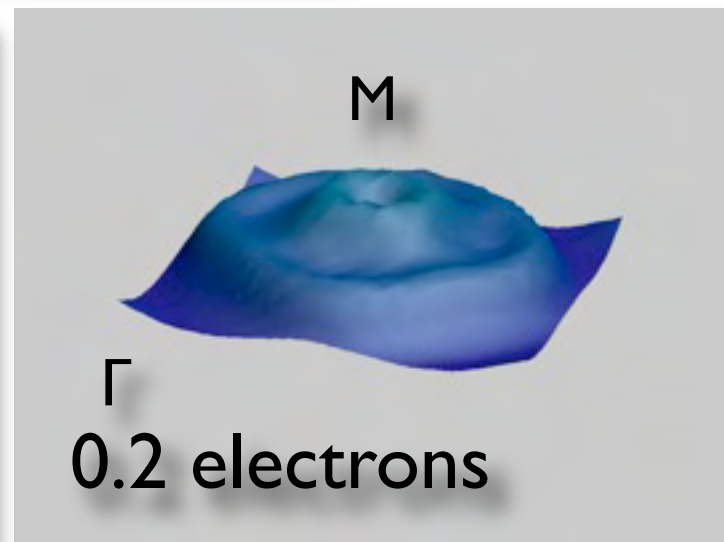
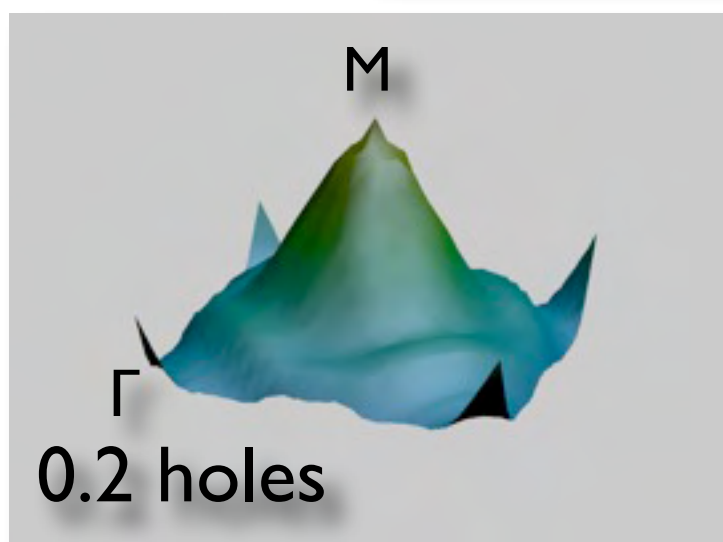


# Nesting in IIII as a function of doping

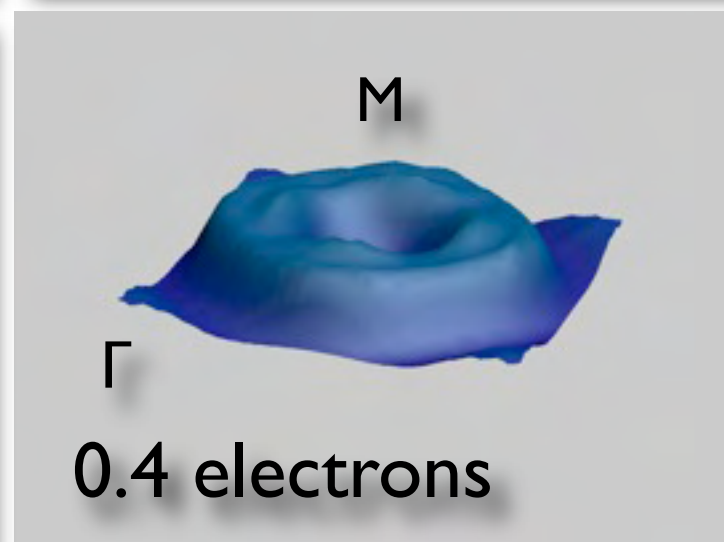
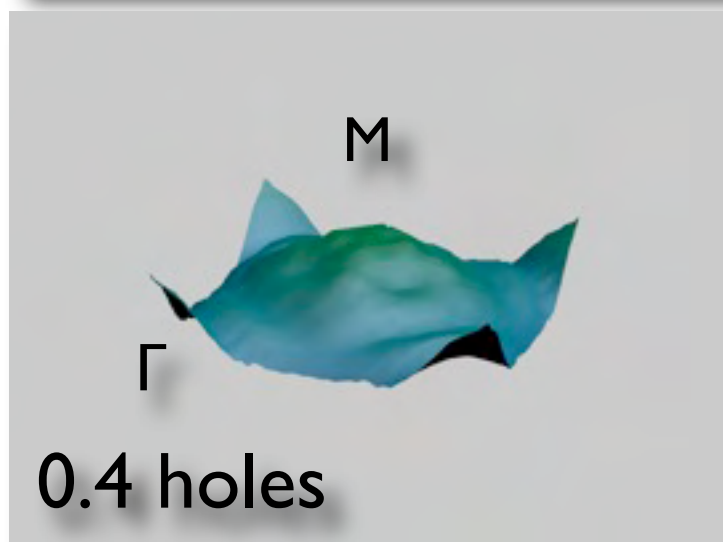
LaFeAsO



The nesting peak decreases with doping.



For SC, it is the total weight of the peak that matters, not the height

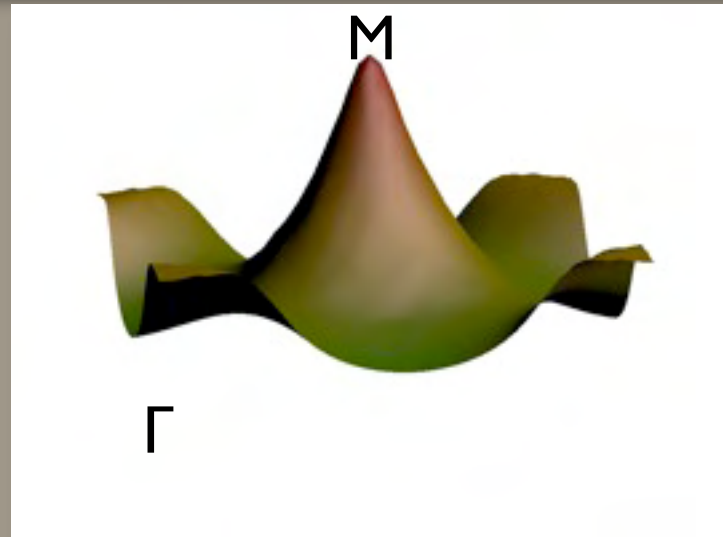




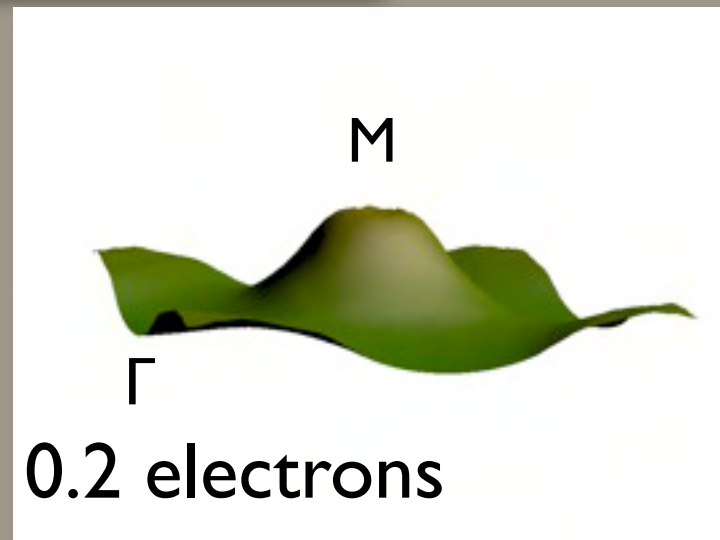
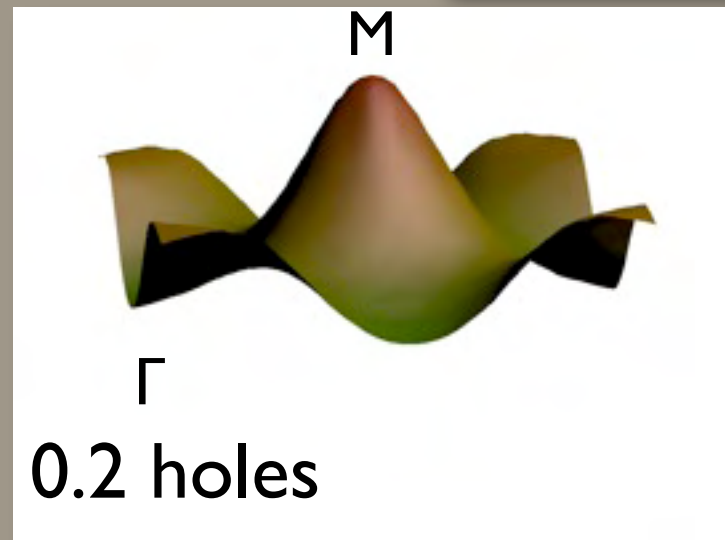


# Magnetic response: $\chi'(q)$ as a function of doping

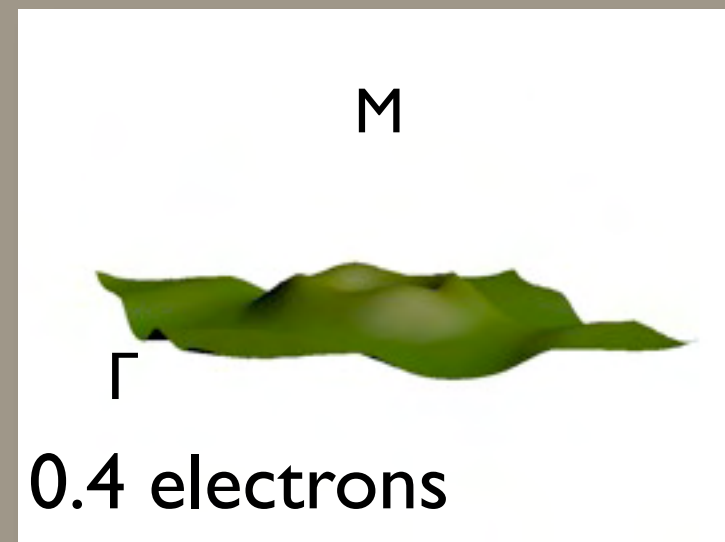
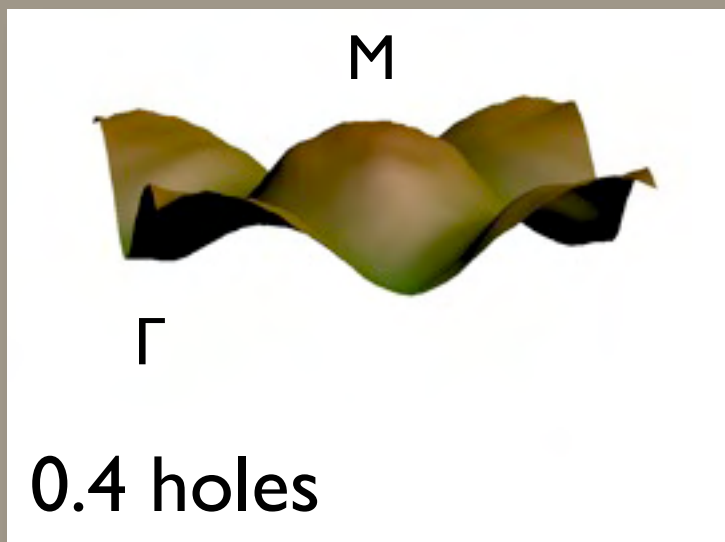
LaFeAsO



The real part of the susceptibility decreases with doping.



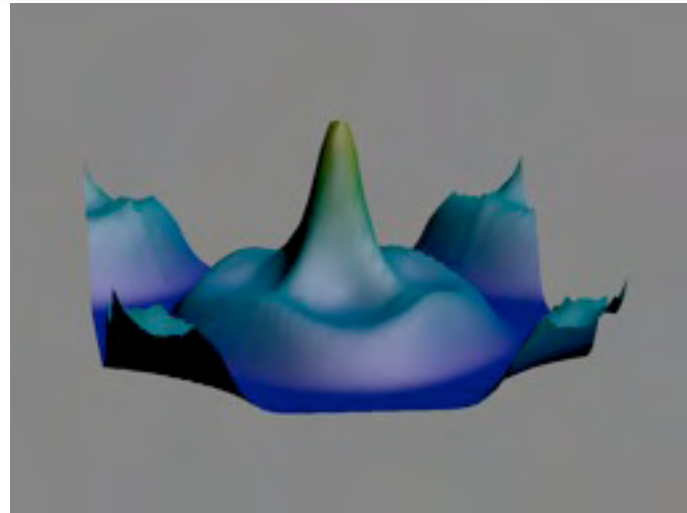
Magnetic transition requires a sharply peaked function





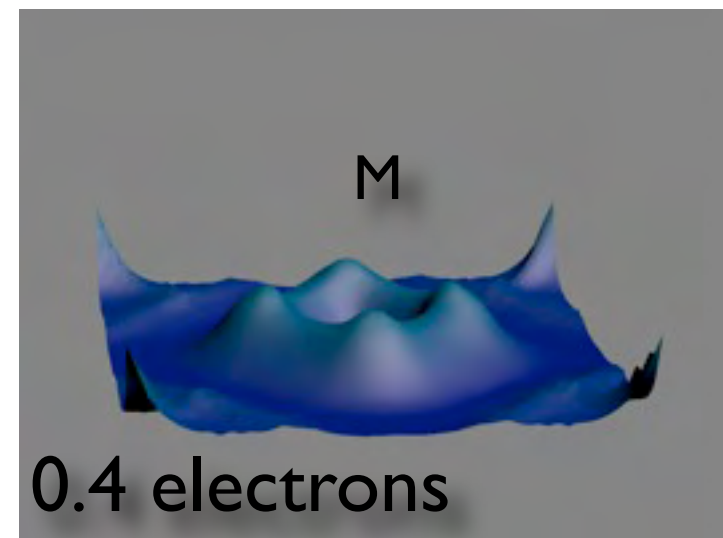
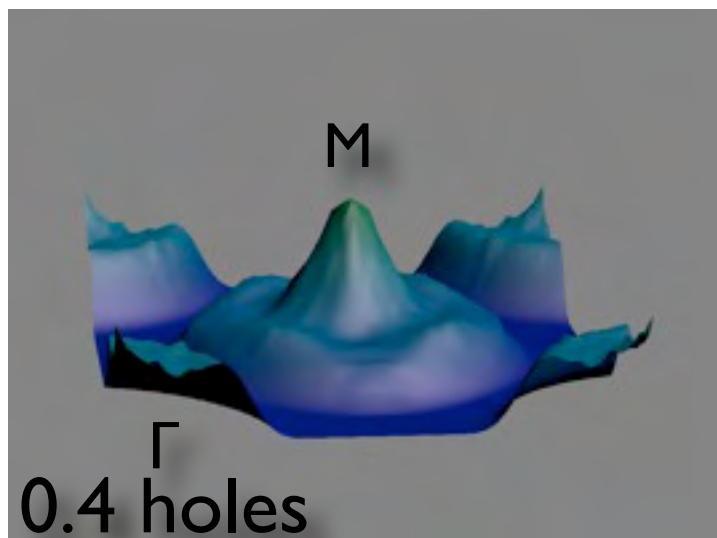
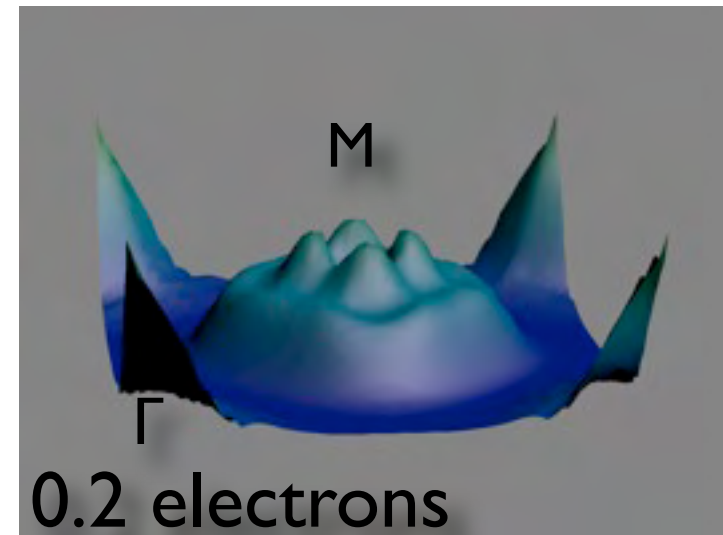
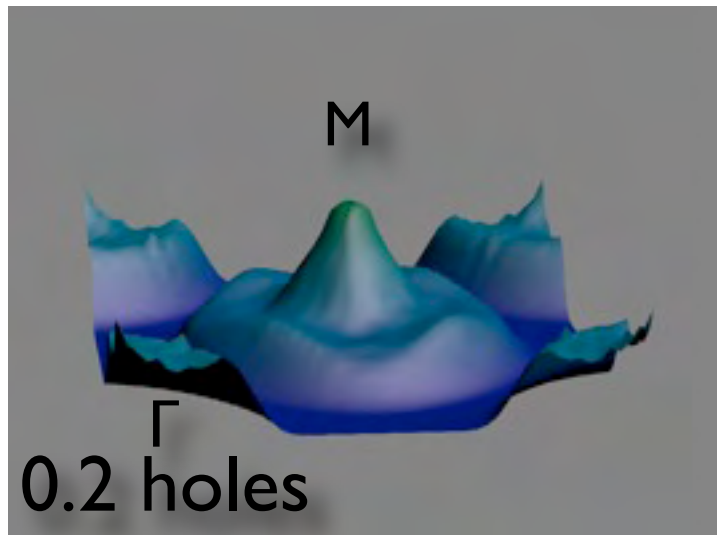


# Nesting in 122 as a function of doping



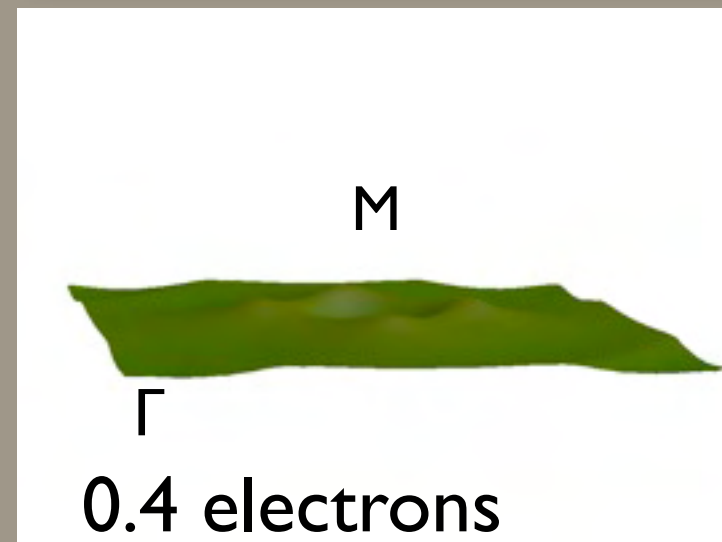
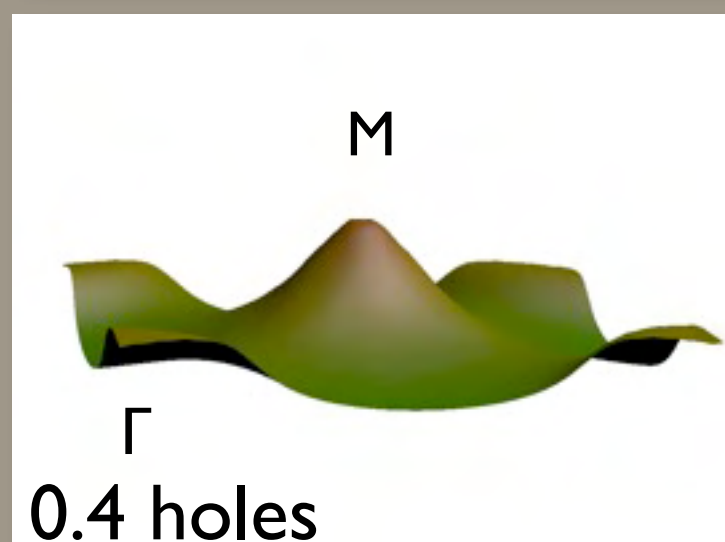
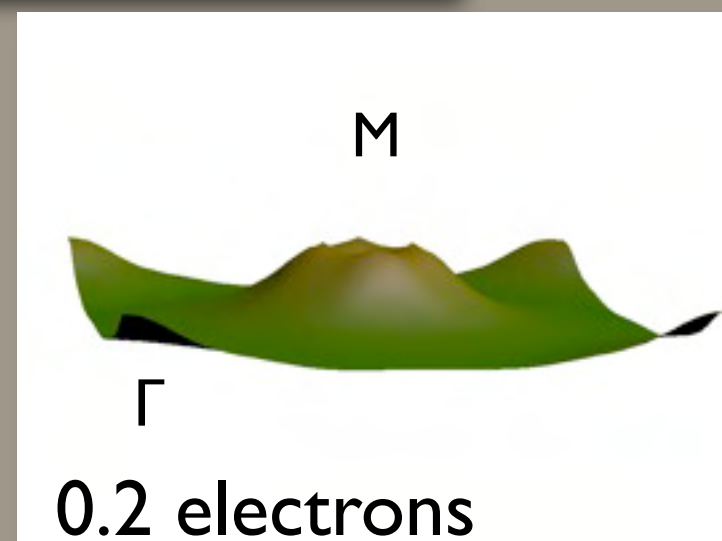
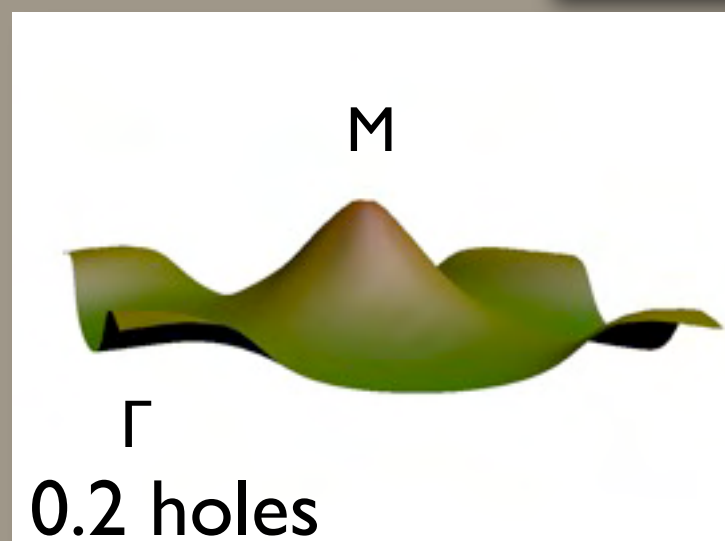
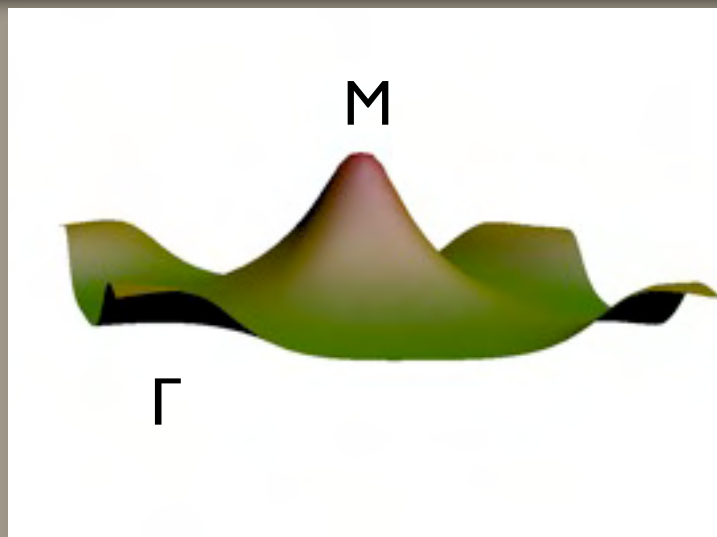
$\text{Ba}_{1-x}\text{K}_x\text{Fe}_2\text{As}_2$

$\text{BaFe}_{2-x}\text{Co}_x\text{As}_2$





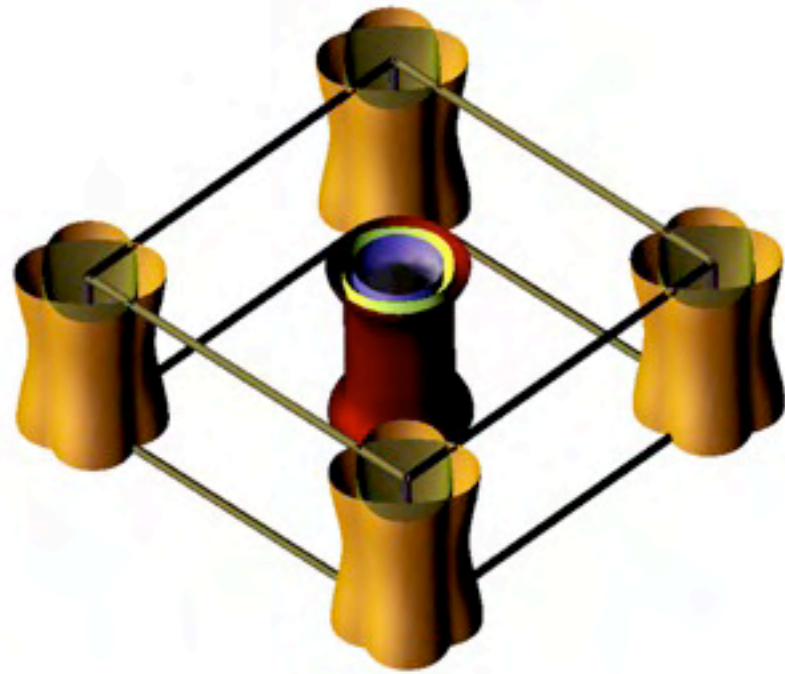
# Magnetic response, $\chi_0'(q)$ , as a function of doping in 122



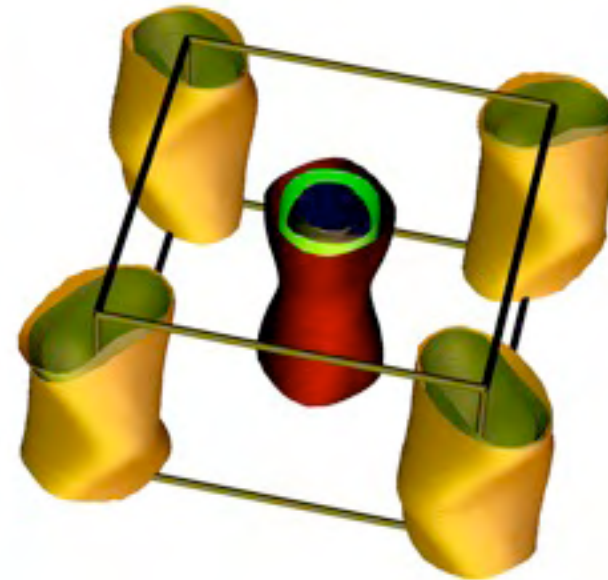


# How does FeTe differ electronically from other structural types?

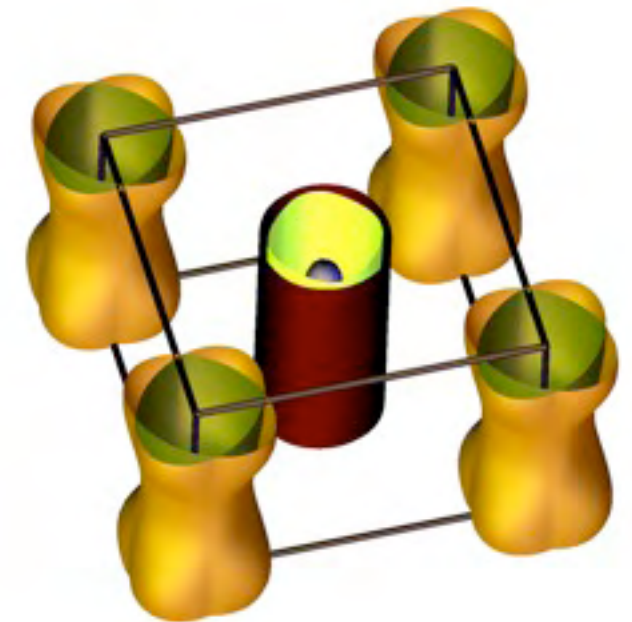
1111



122



FeTe



FeTe is isoelectronically doped (with Se) to achieve superconductivity

FeTe Fermi surface is extremely similar to LaFeAsO and BaFe<sub>2</sub>As<sub>2</sub> surfaces.

Nesting properties should also be very similar

Re  $\chi_0$  could differ (DOS away from  $E_F$  shows significant differences)

Theory: real part of susceptibility drawn from wide energy range will peak at the double stripe wave vector



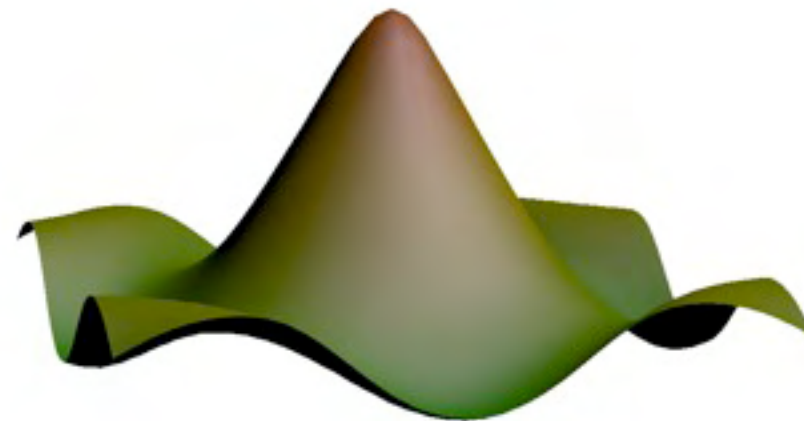
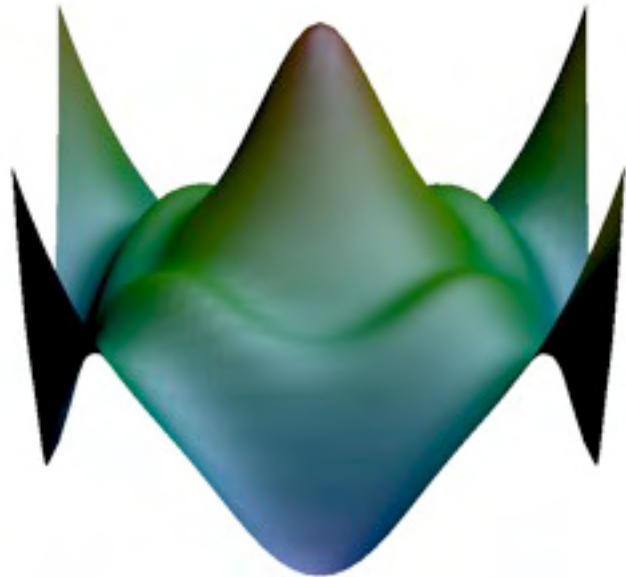


# Are the calculable properties different in FeTe?

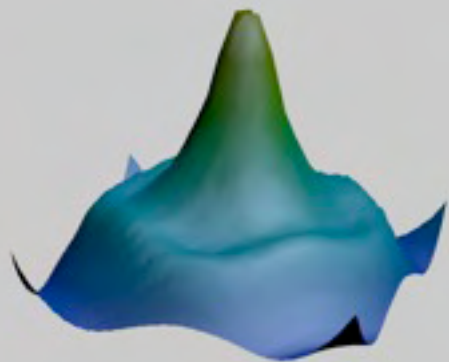
Nesting function

Real part of susceptibility

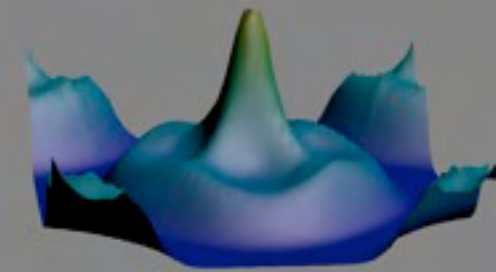
FeTe



Comparison to 1111, 122 systems:



LaFeAsO



BaFe<sub>2</sub>As<sub>2</sub>

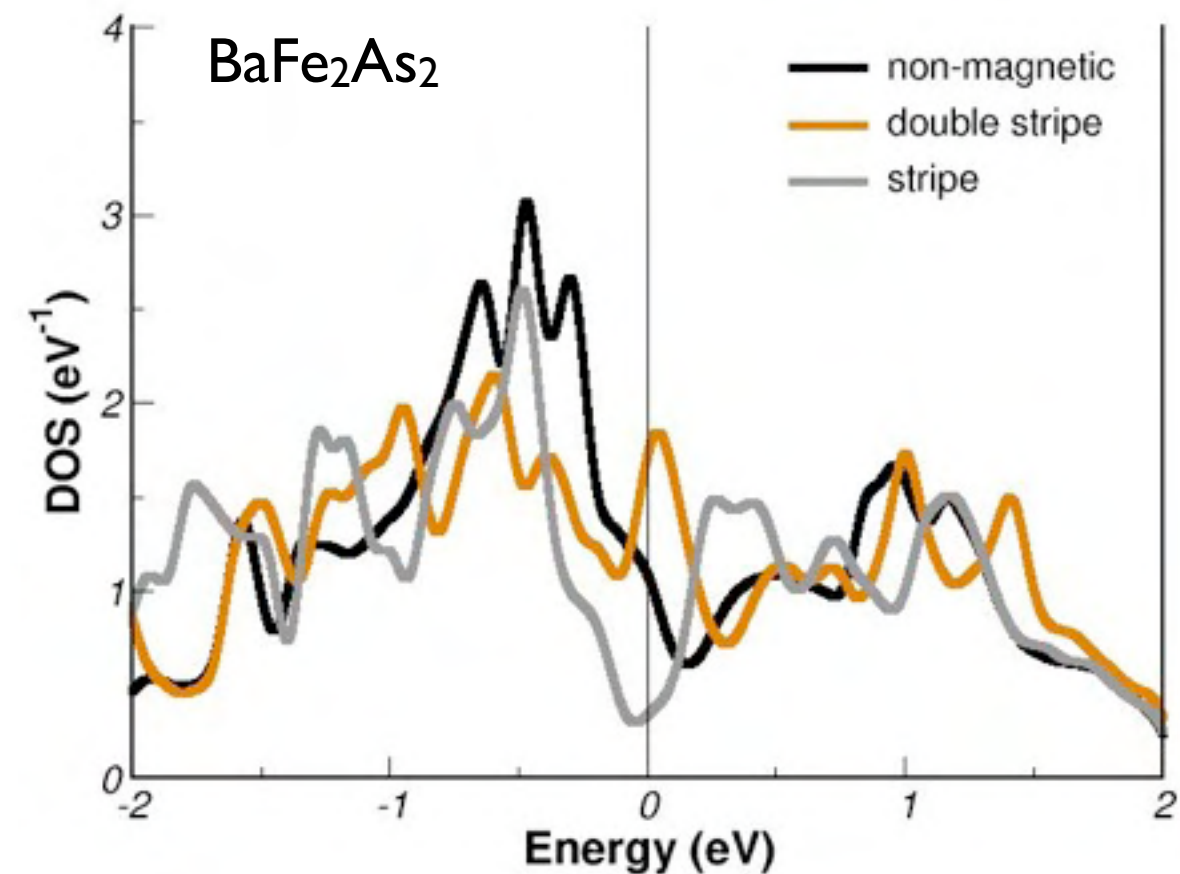


FeTe shows no very different nesting or tendency toward magnetic instability

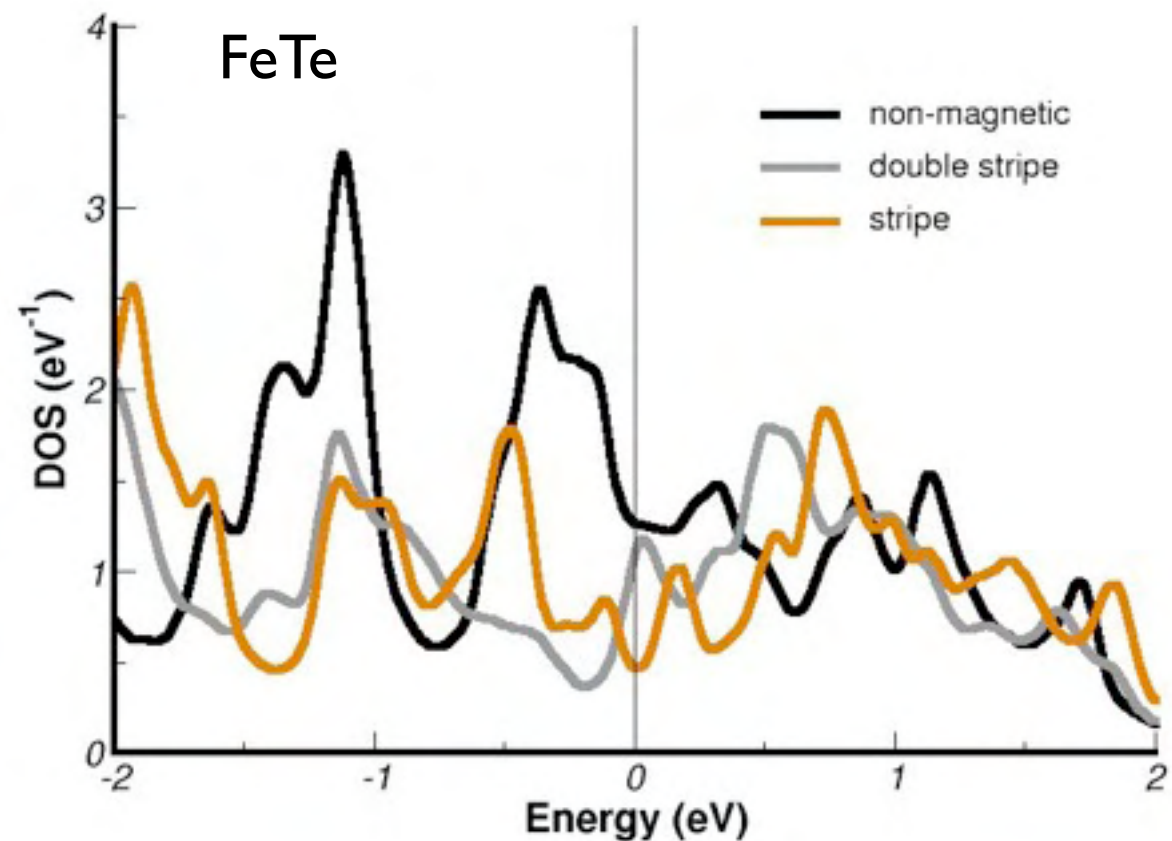




# Energy gain away from the Fermi energy



Ground state: stripe



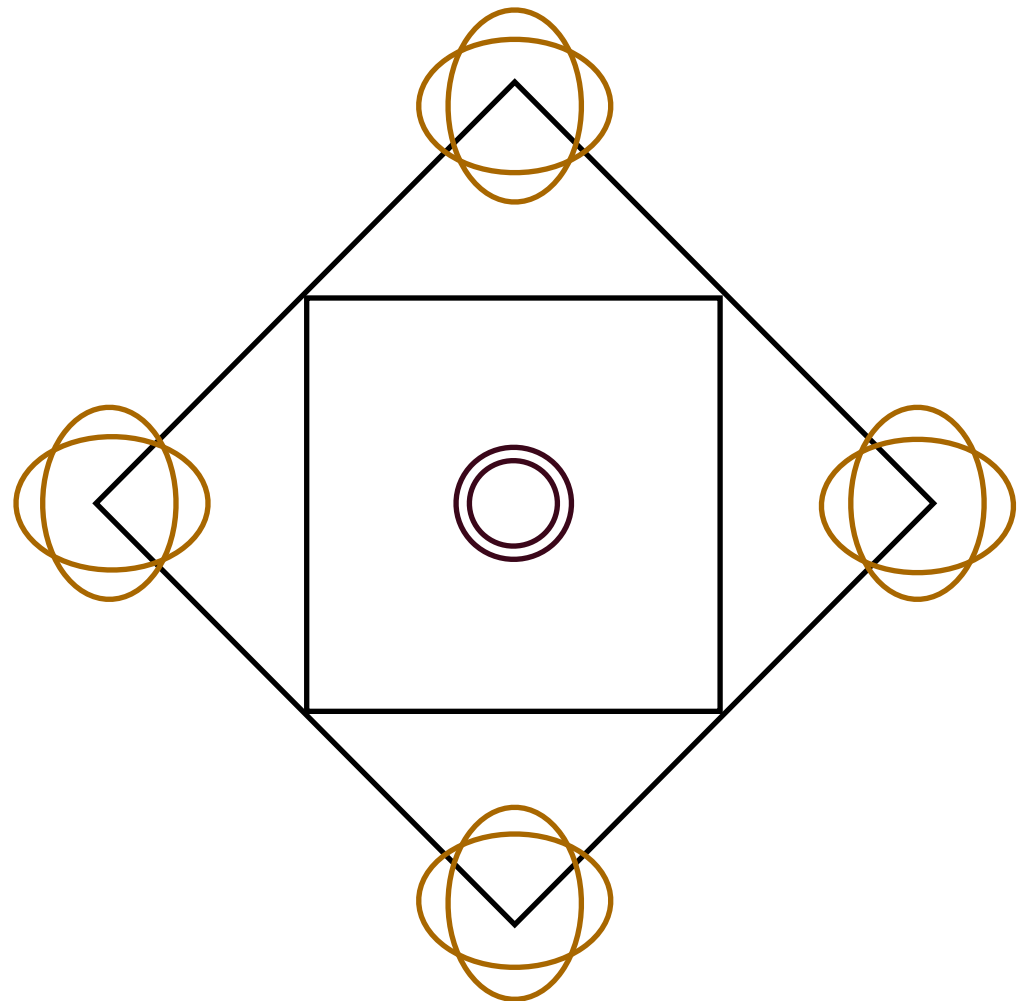
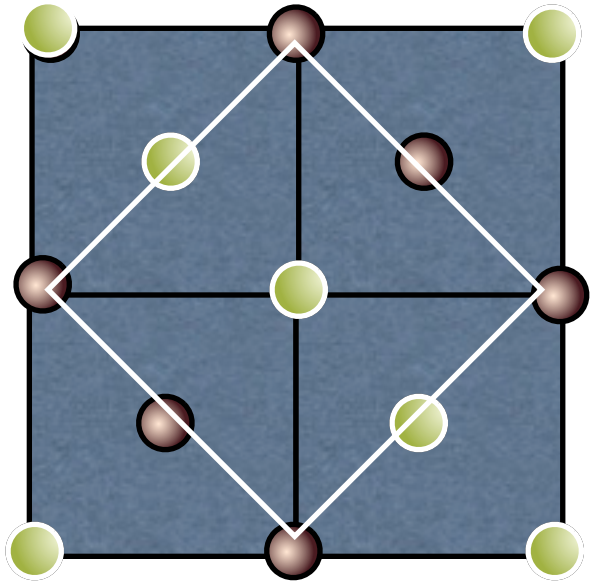
Ground state: double stripe

Ground state of both structure types is achieved through lowering of one-electron energies over a wide range



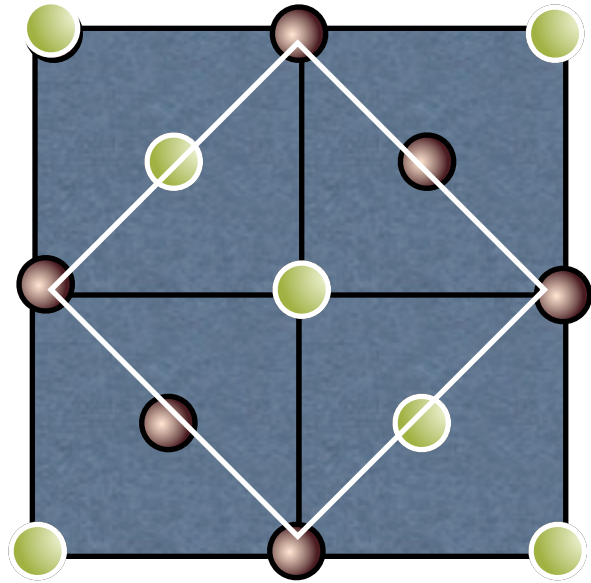
# Magnetic ordering is electronically dramatic

LaFeAsO

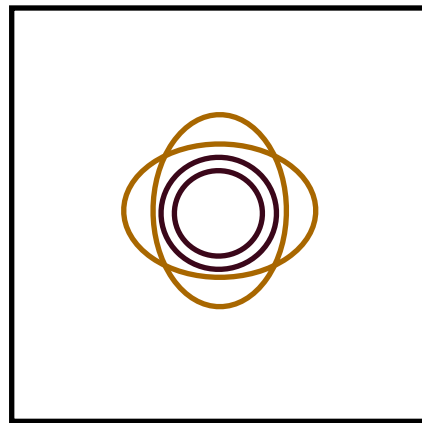
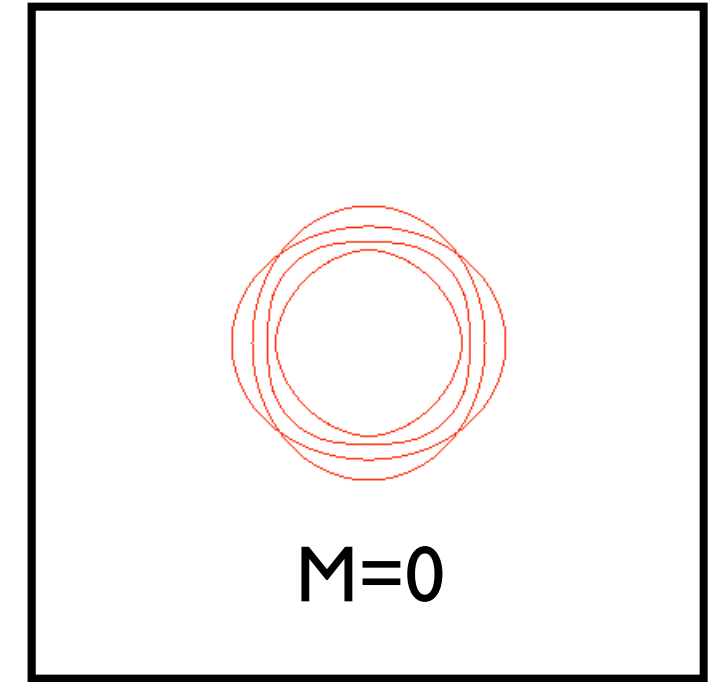
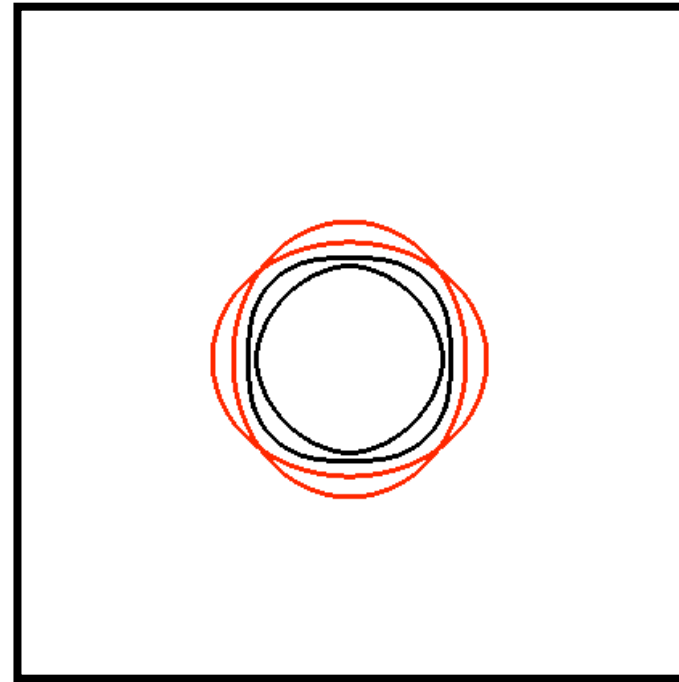




# Magnetic ordering is electronically dramatic

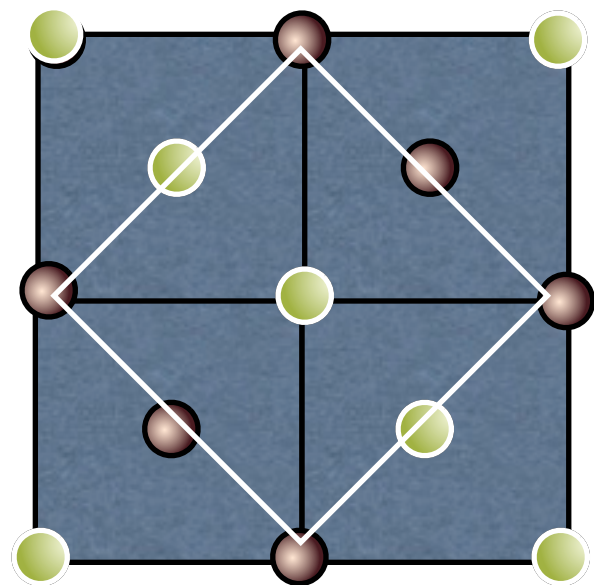


LaFeAsO

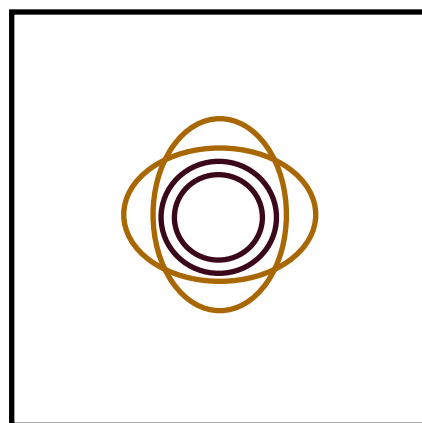
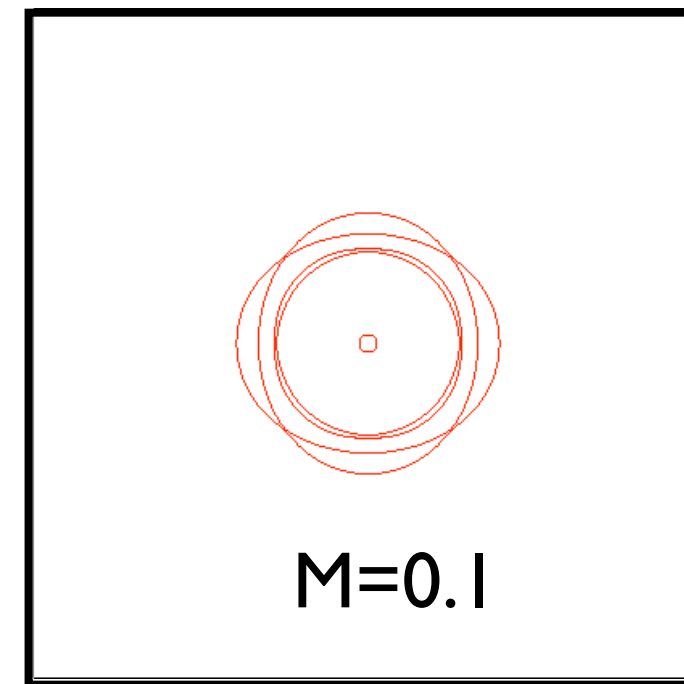
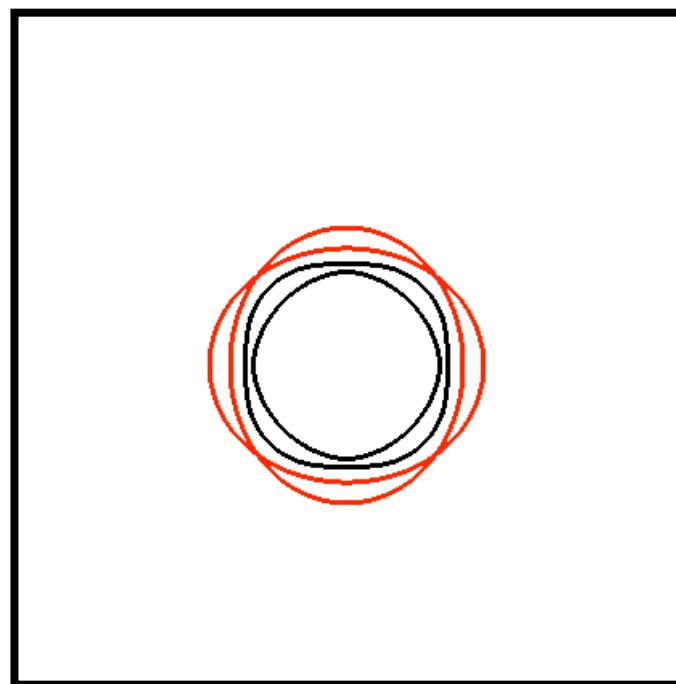




# Magnetic ordering is electronically dramatic



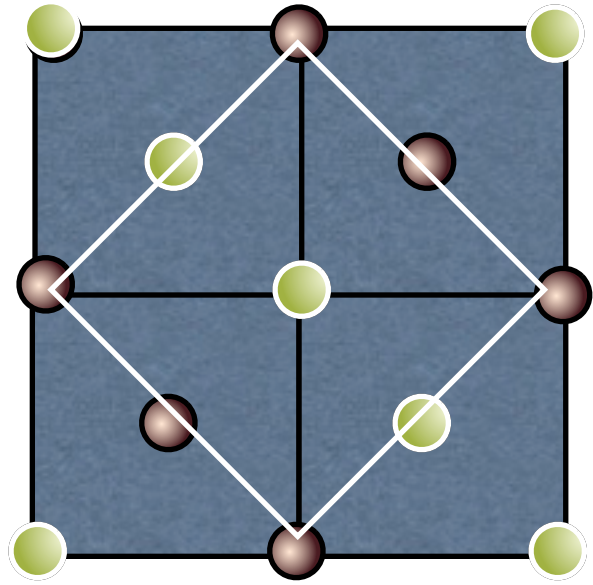
LaFeAsO



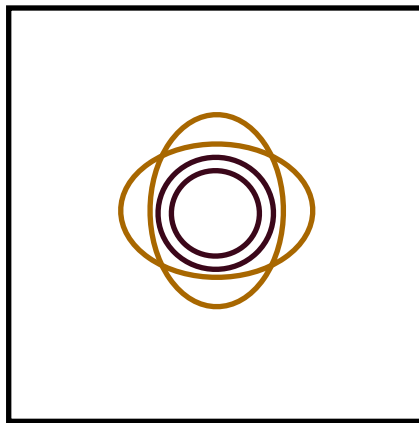
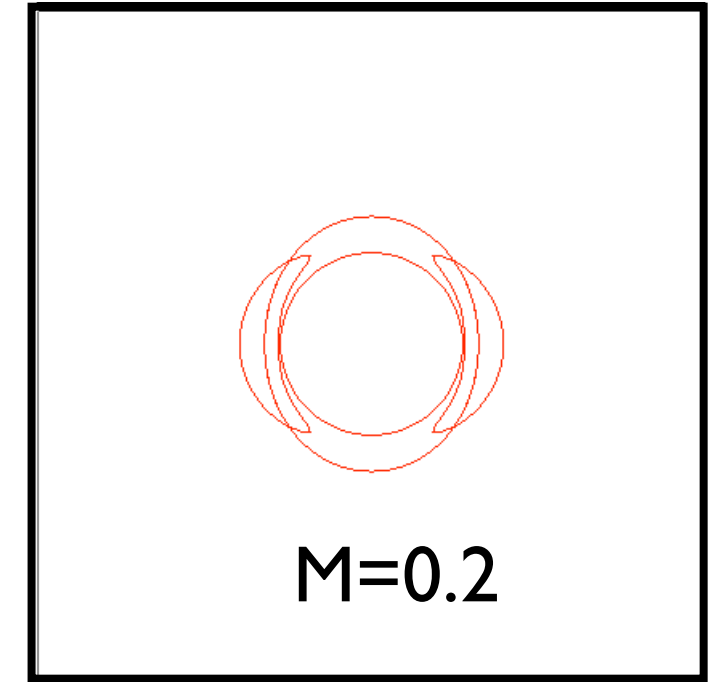
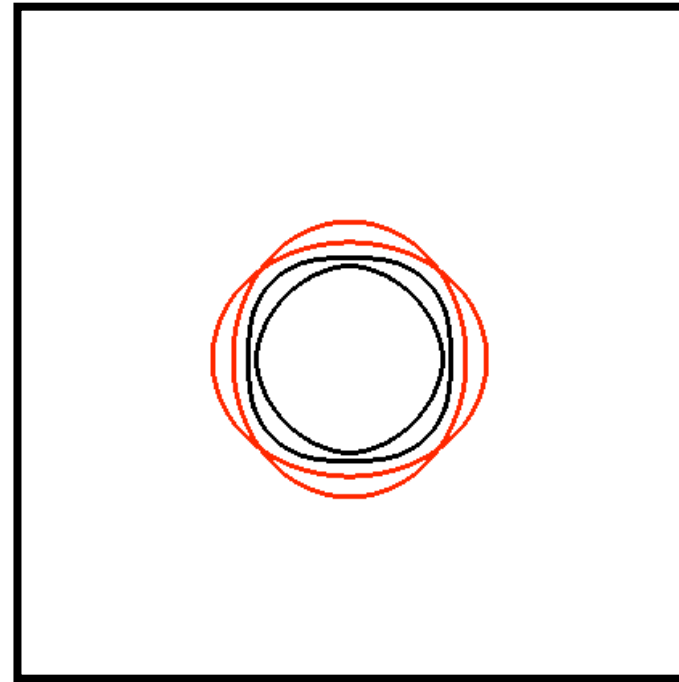




# Magnetic ordering is electronically dramatic

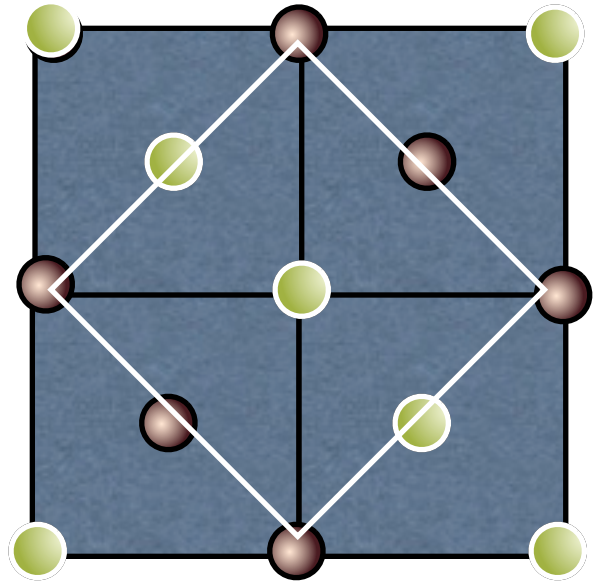


LaFeAsO

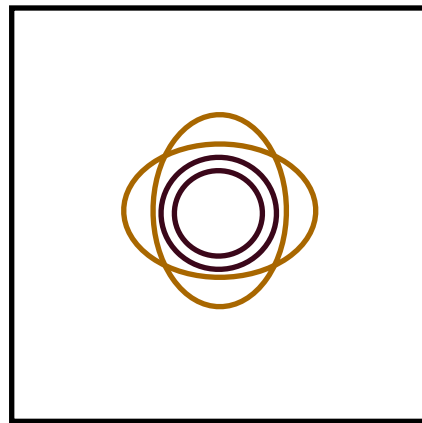
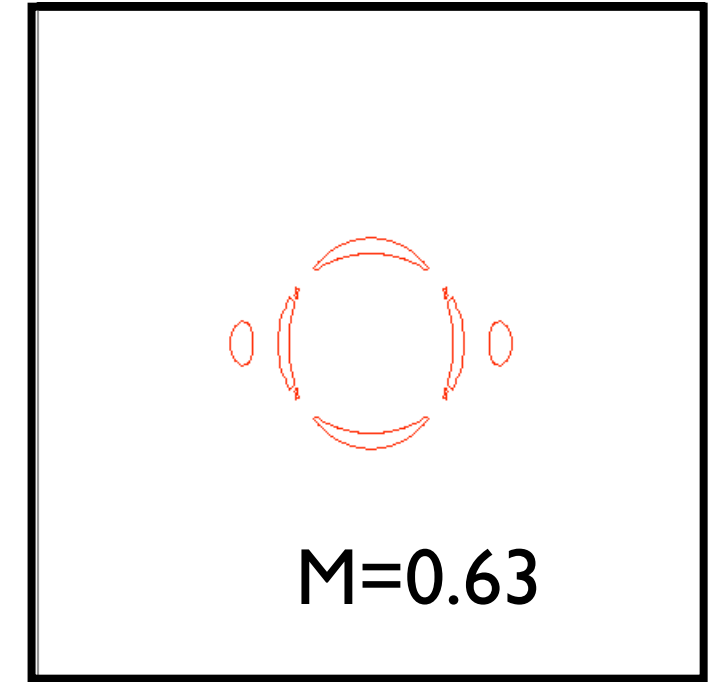
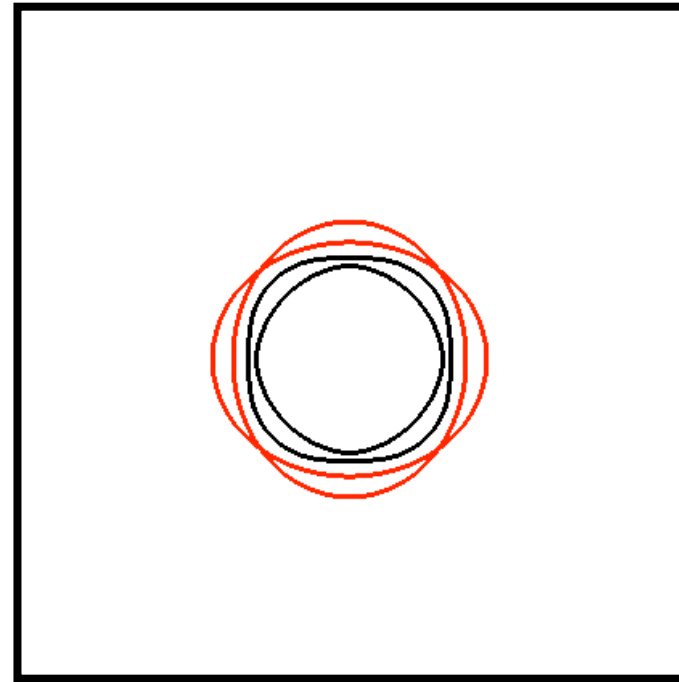




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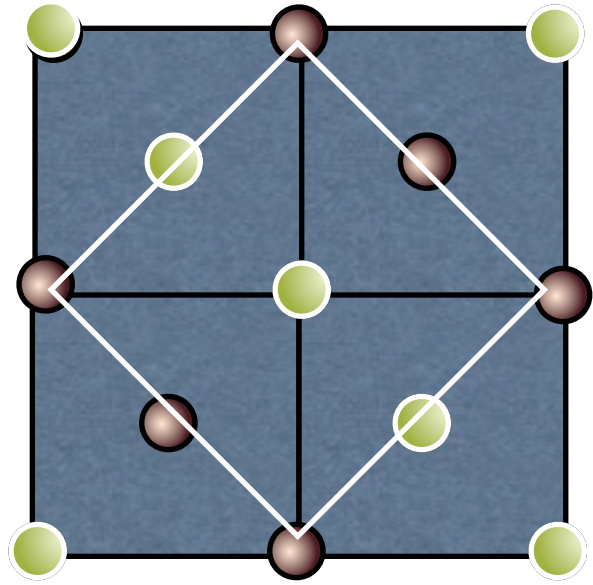


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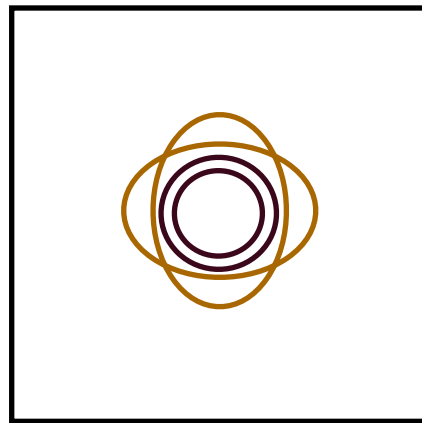
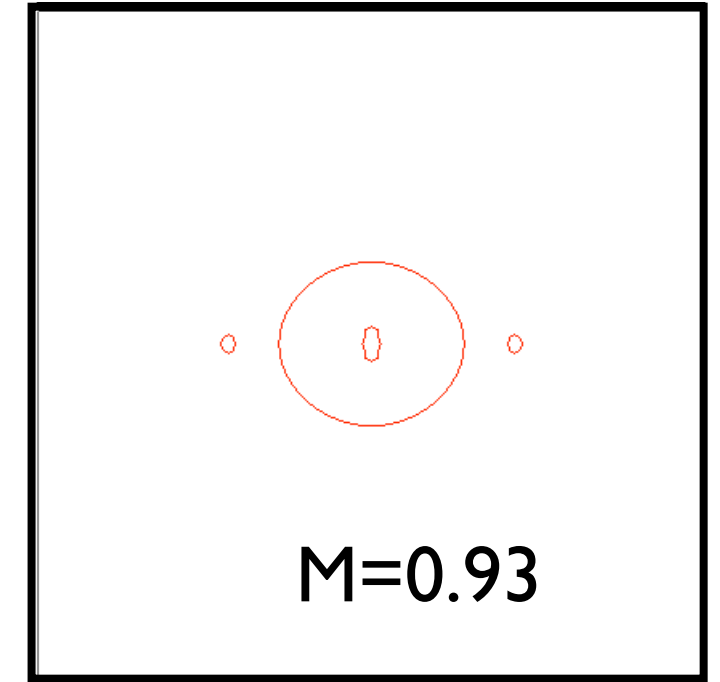
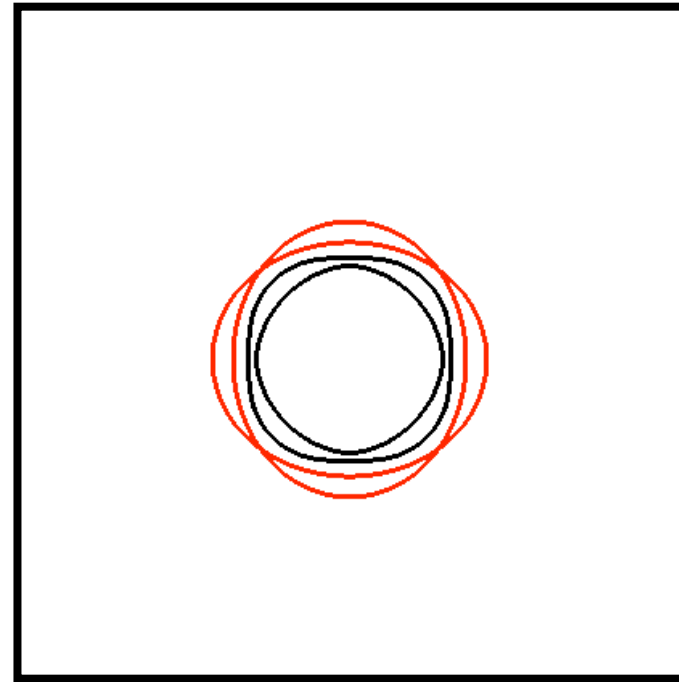




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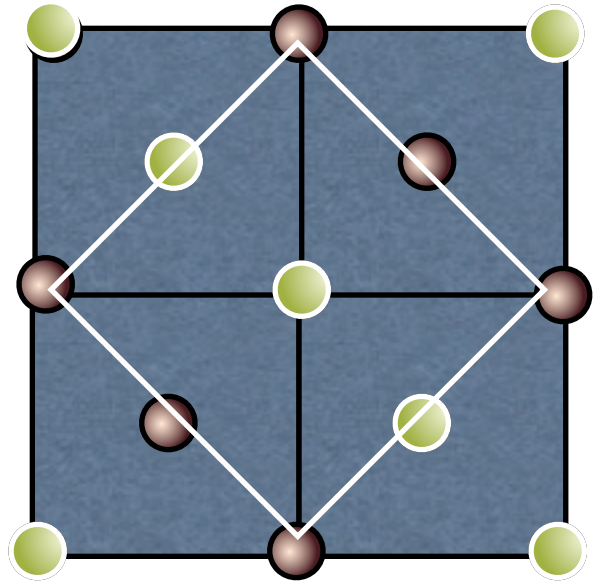


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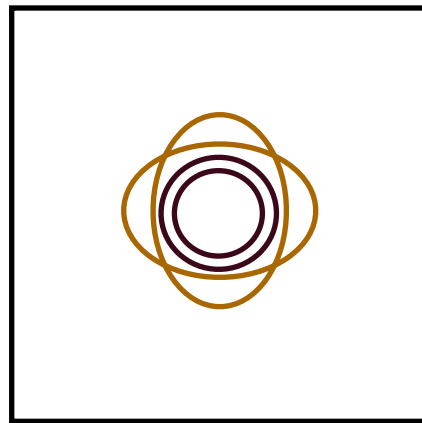
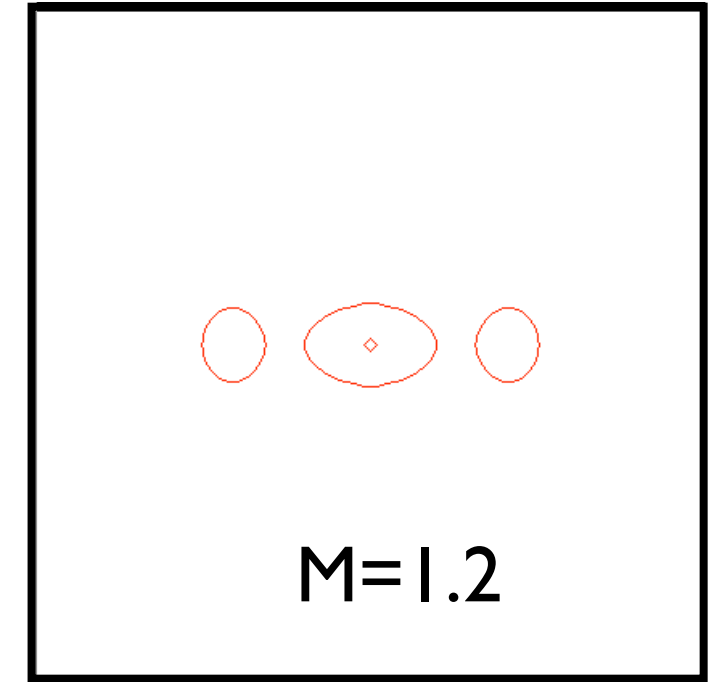
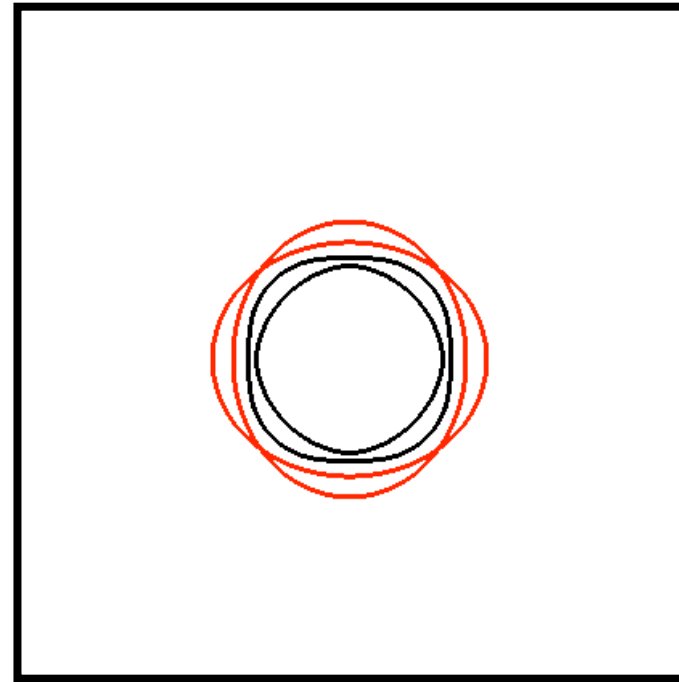




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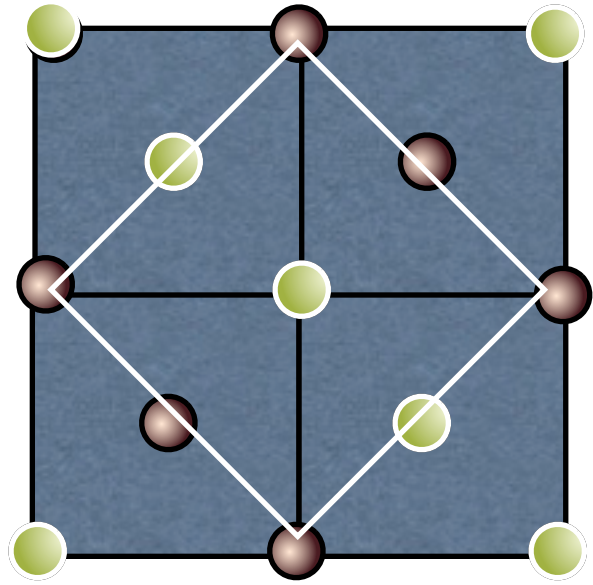
LaFeAsO



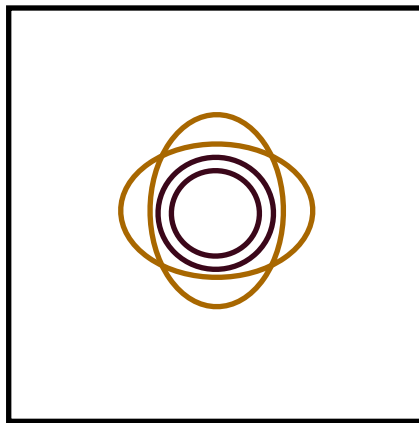
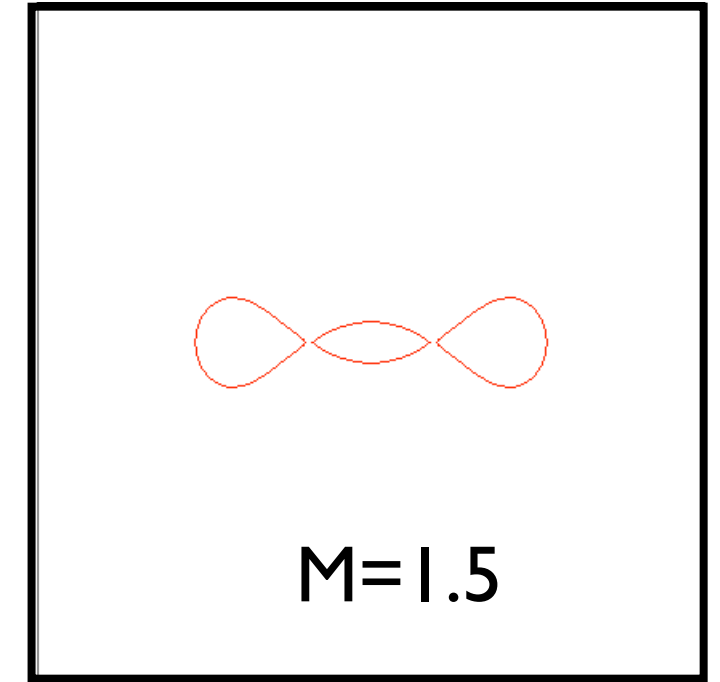
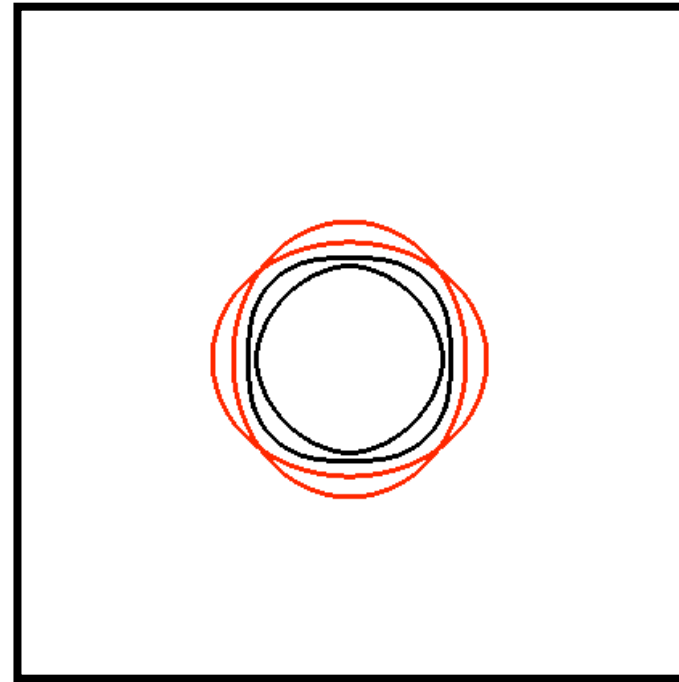




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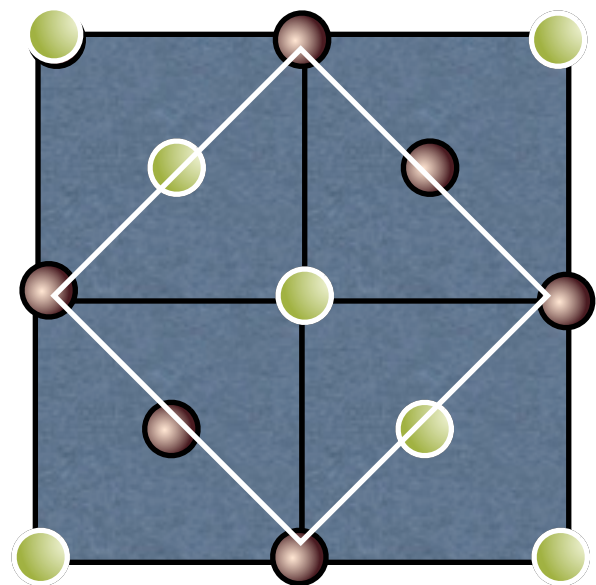


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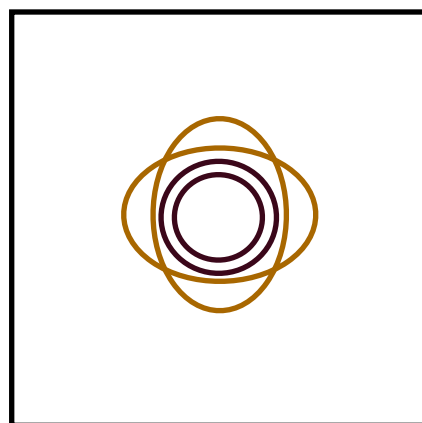
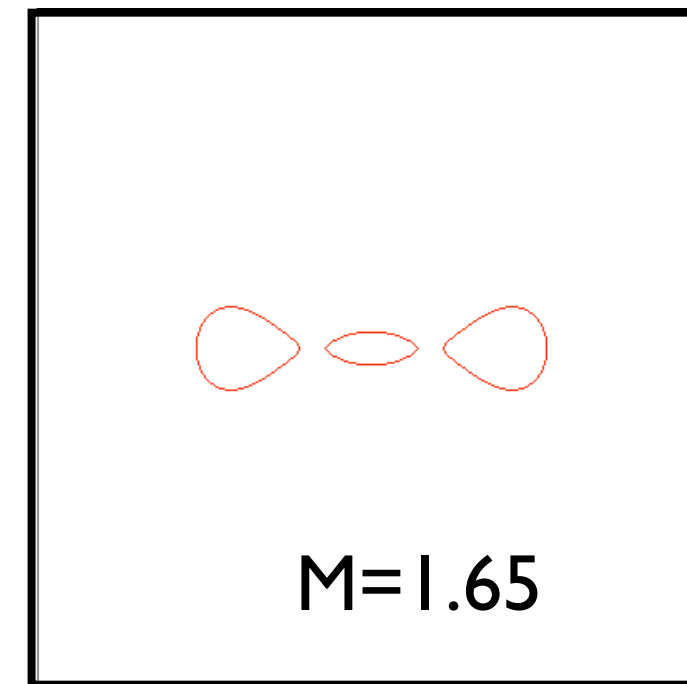
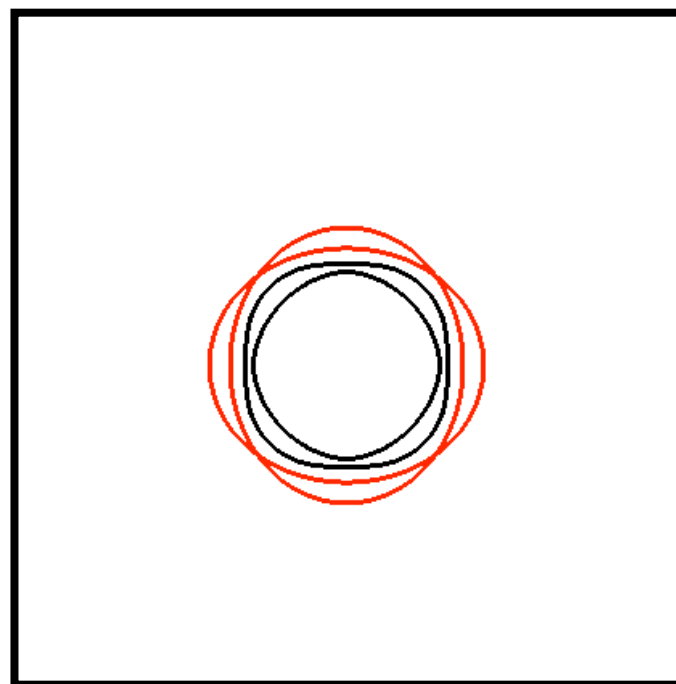




# Magnetic ordering is electronically dramatic

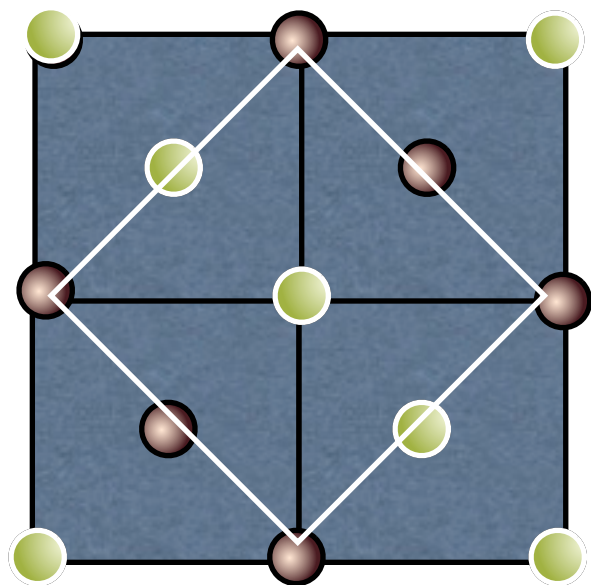


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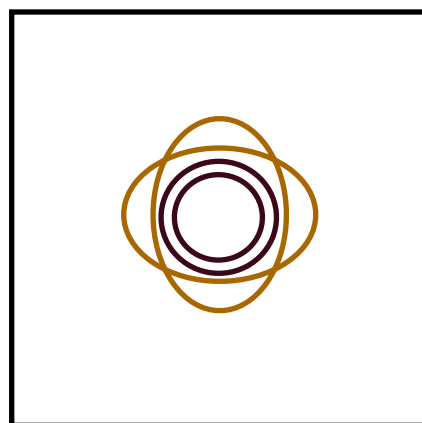
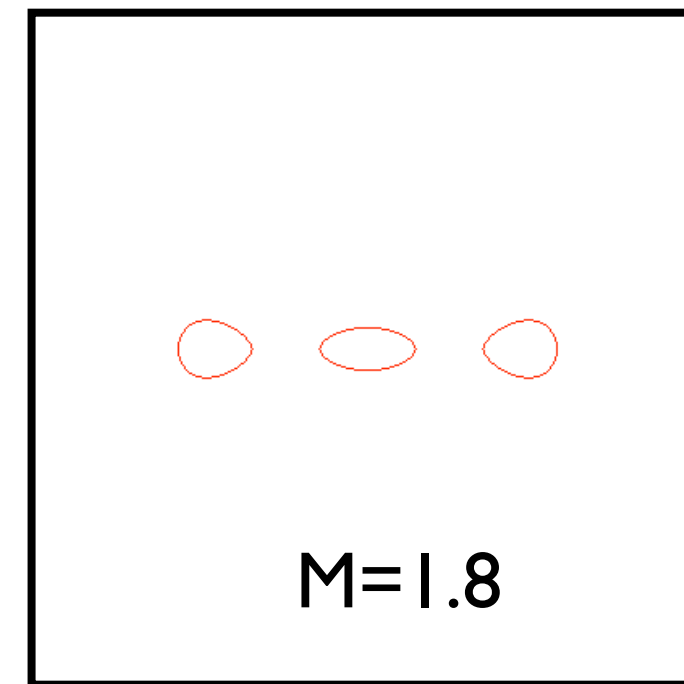
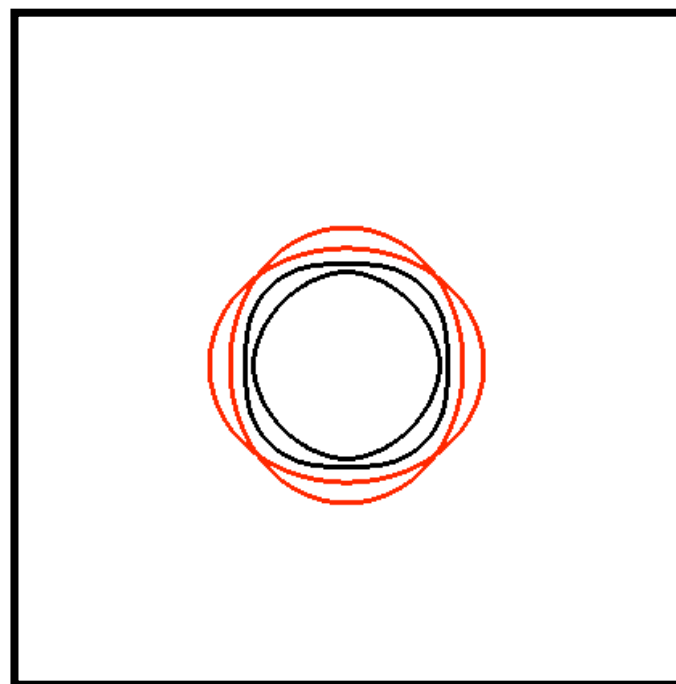




# Magnetic ordering is electronically dramatic



LaFeAsO

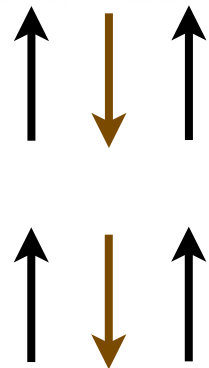
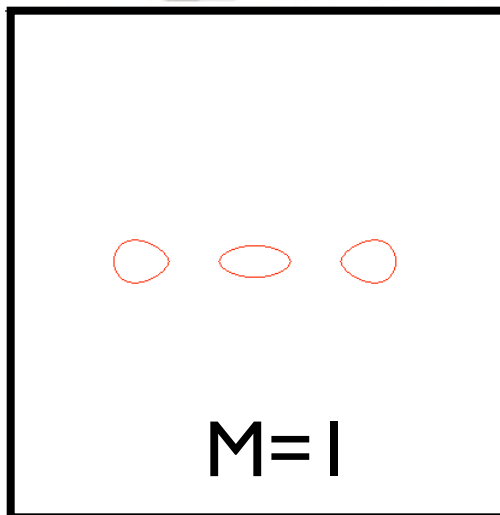
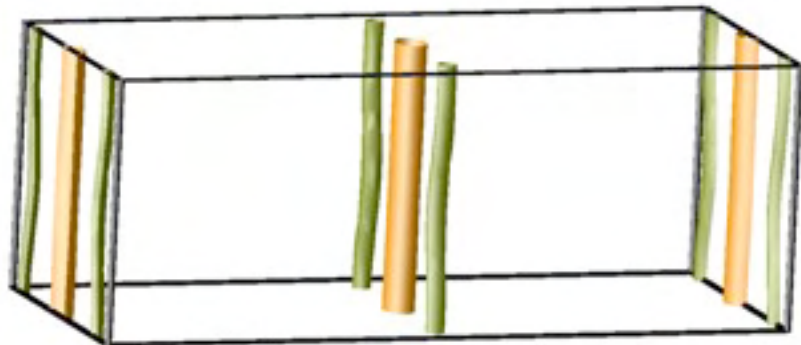


- Magnetism is not a small shift of bands
- Linear scheme suggested by  $\chi_0(q,0)$  may be inappropriate (*is for FeTe at least*)
- Look elsewhere for 'trigger' that establishes/destroys order

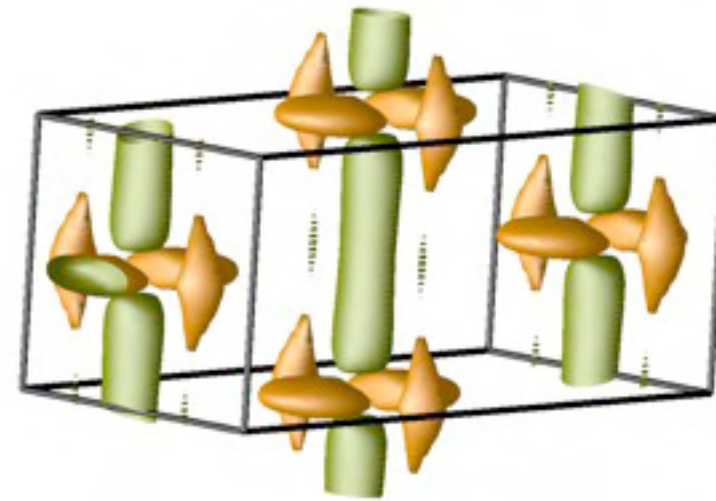


# Magnetic Fermi Surfaces

1111



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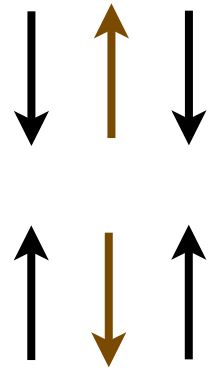
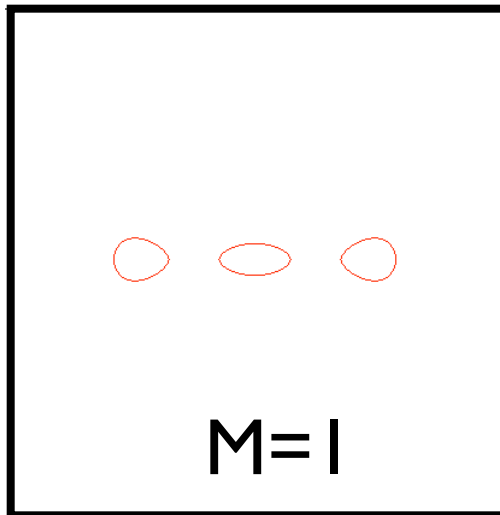
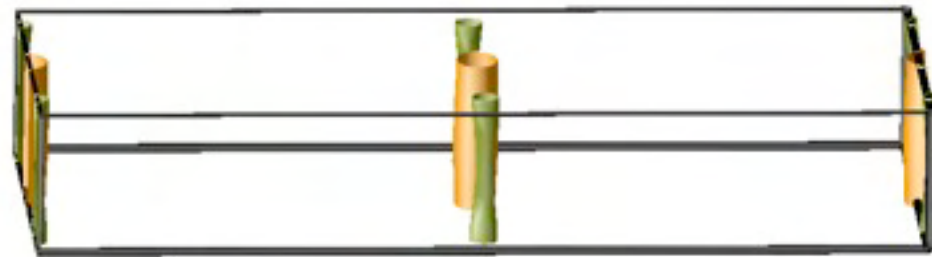
What is the 'trigger' that establishes/destroys order?



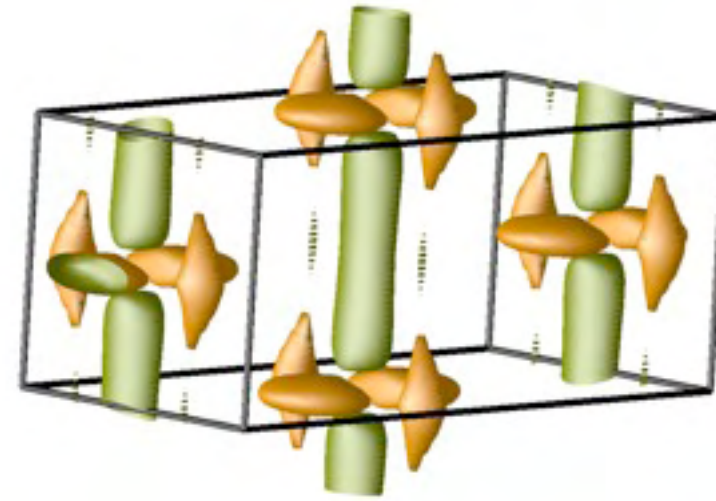


# Magnetic Fermi Surfaces

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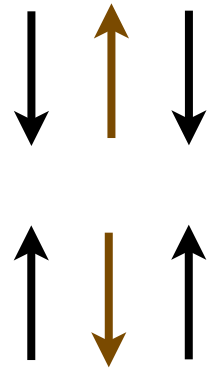
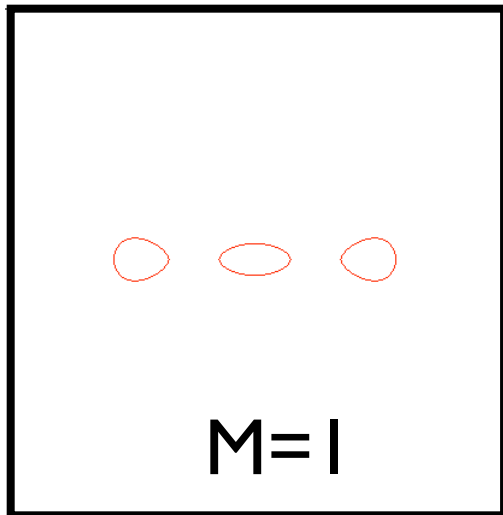
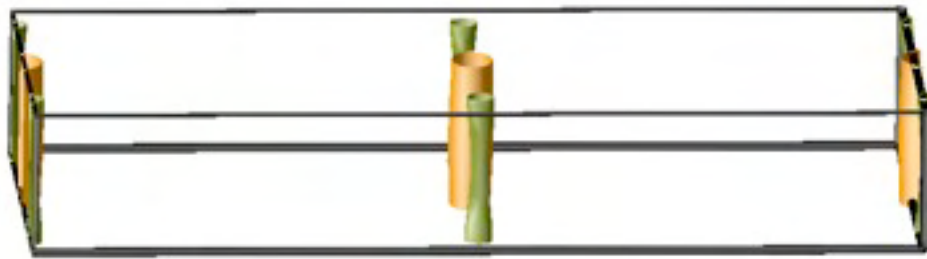


What is the 'trigger' that establishes/destroys order?

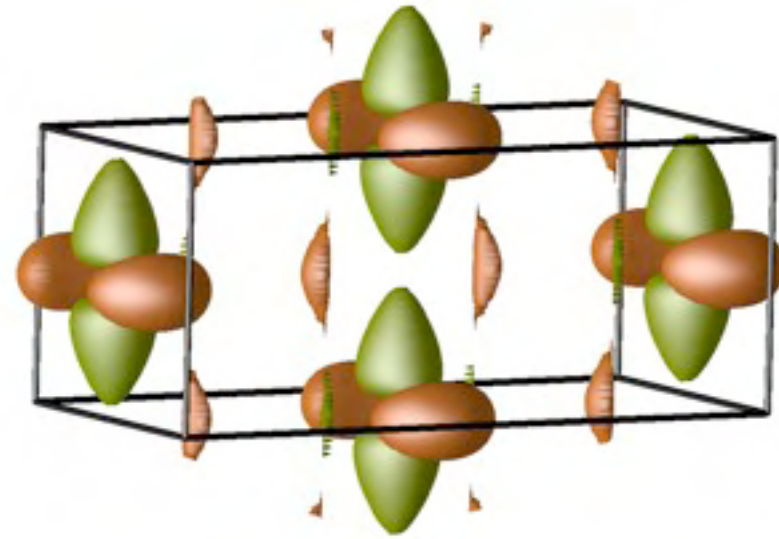


# Magnetic Fermi Surfaces

1111



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Clear differences exist between the structural types in terms of *magnetic* Fermi surfaces

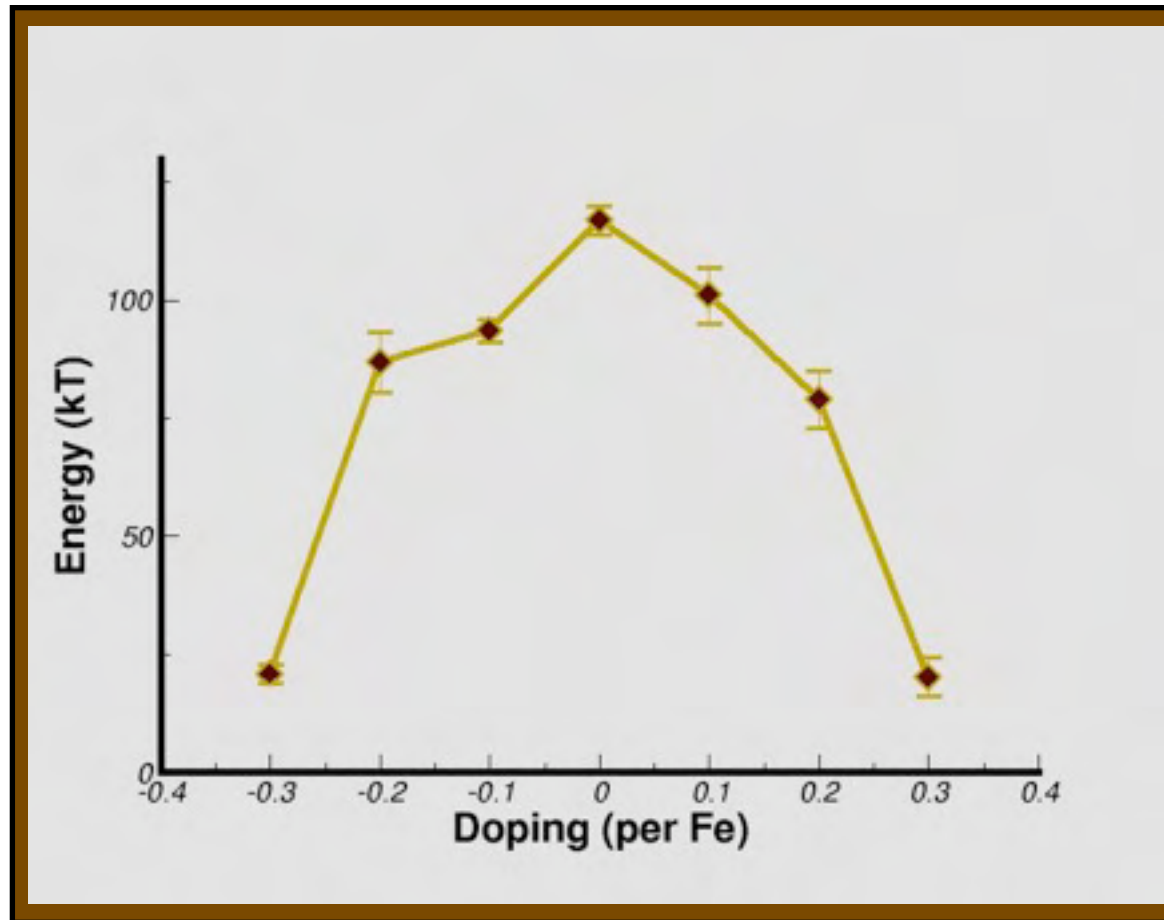
What is the 'trigger' that establishes/destroys order?



# What fundamentally controls long-range order?

In 2D, spin fluctuations prevent LRO above  $T=0$  (Mermin-Wagner)

Degree of three-dimensionality could be key to ordering

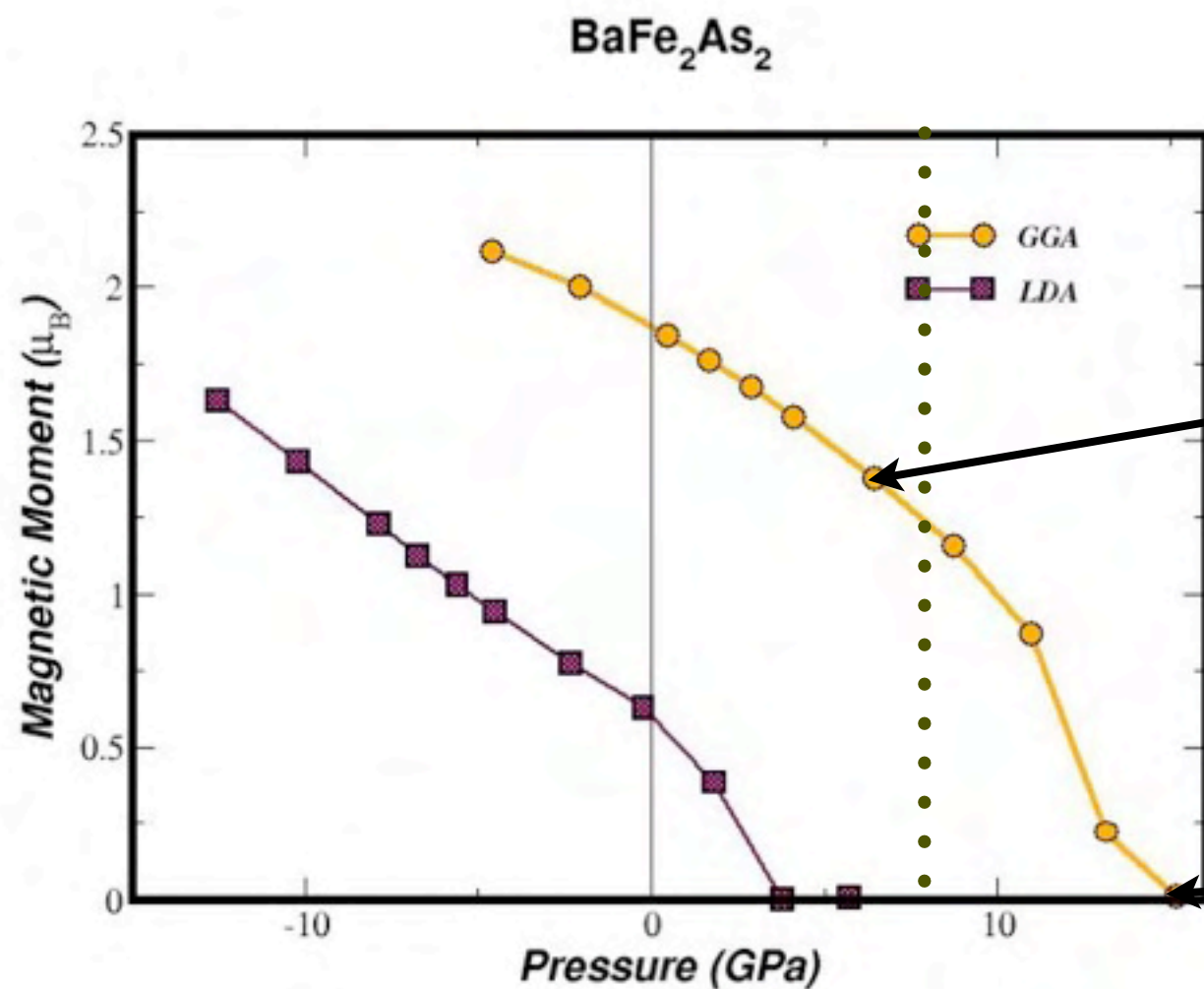


- Coupling between planes dies off with both hole and electron doping
- Energy scale is commensurate with ordering temperature

But, what about pressure-induced SC?



# Pressure dependence of magnetism



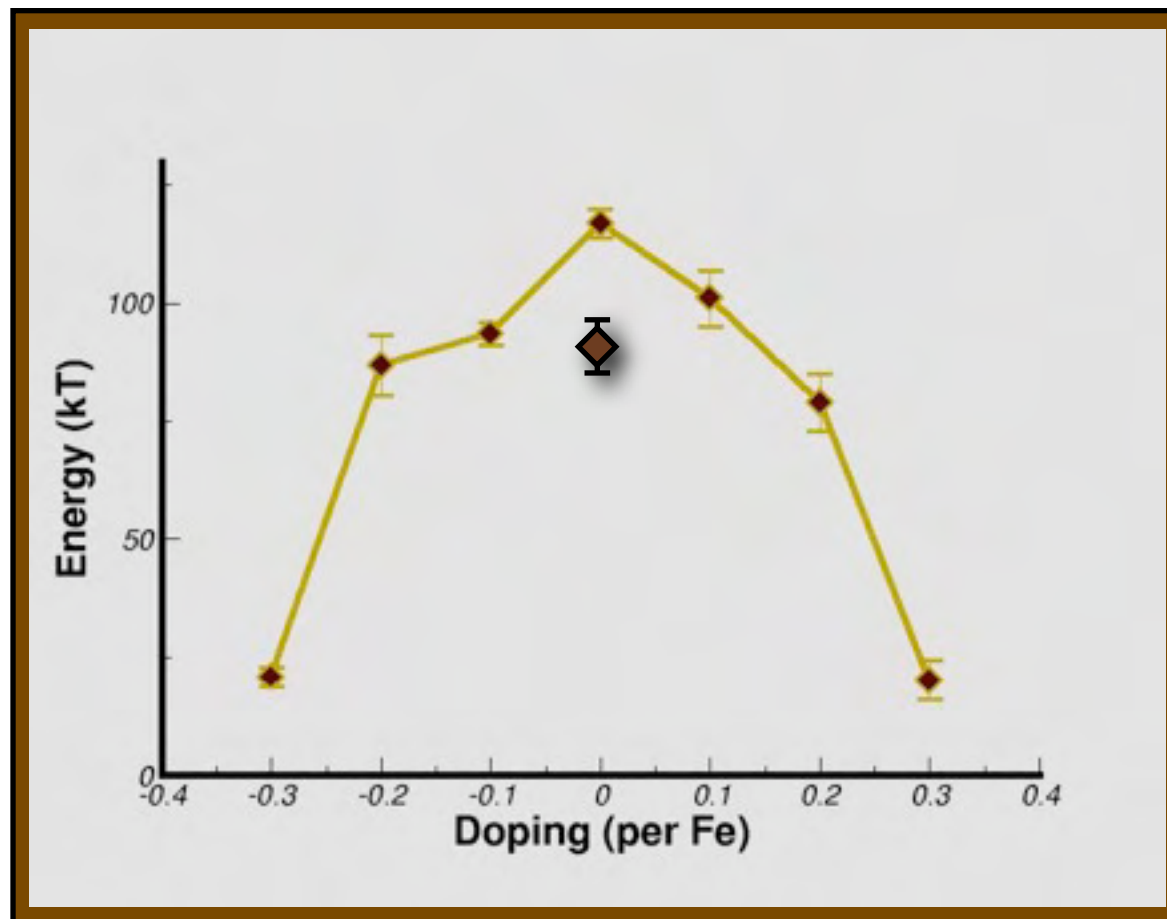
Pressure of 6.7 GPa, reduces magnetic moment from  $2.1 \mu_B$  to  $1.38 \mu_B$

Pressure of 15 GPa, reduces magnetic moment to zero





# Pressure dependence of magnetism



Pressure of 6.7 GPa, reduces magnetic moment from  $2.1 \mu_B$  to  $1.38 \mu_B$

Pressure of 15 GPa, reduces magnetic moment to zero

Coupling reduced by 25%

Reduced moment translates to reduced interplanar coupling, despite compressed interplanar distance



## Summary

- Magnetism and superconductivity are strongly interrelated in Fe pnictides (and chalcogenides)
- Long range establishment of SDW must be suppressed for SC to appear
- Magnetism is *not* nesting driven; not superexchange either
- Key to suppressing SDW may be interplanar coupling

What can be learned from non-magnetic electronic structure?

Which are the relevant electronic states to consider for superconductivity? (s<sup>+/-</sup> picture derived from non-magnetic FS)