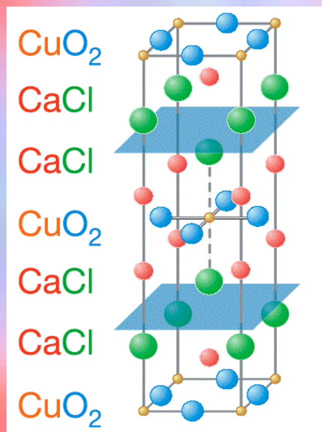
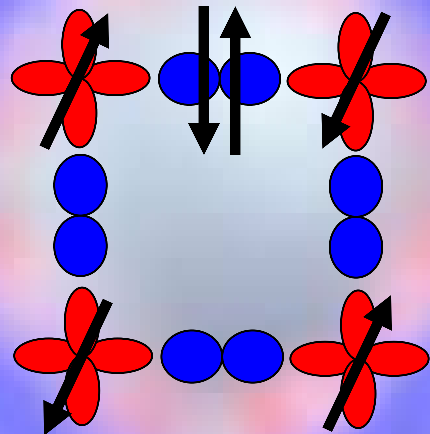
Nature of Striped Phases in Cuprates with x ~ 1/8



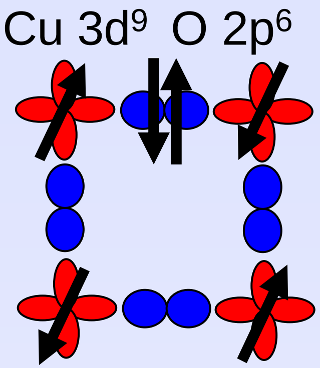


Charles H. Patterson
School of Physics
Trinity College Dublin

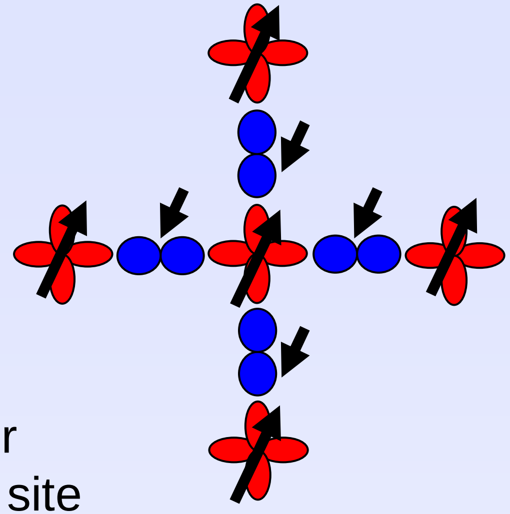
Summary

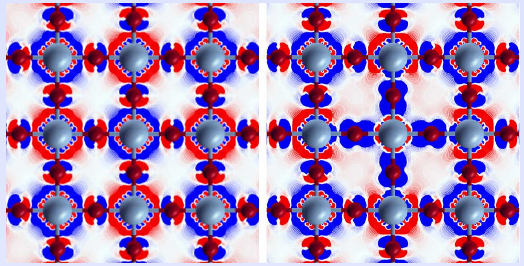
- Hybrid DFT calculations for $Ca_2CuO_2Cl_2$
  - Electronic structure
- Magnetic anti-phase boundaries in $Na_xCa_{2-x}CuO_2Cl_2$ x=1/8
  - Electronic structure
  - STM and STS data
- Small polarons in low-doped $Na_xCa_{2-x}CuO_2Cl_2$ x=1/32
  - Polaron distortions
  - Electronic structure
  - Photoemission

Electronic and Crystal Structures



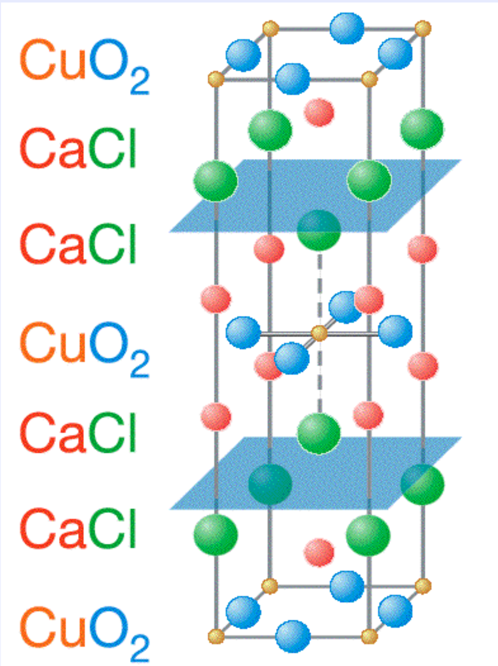
Undoped cuprate
Anti-ferromagnetic insulator
Half-filled 3d x^2-y^2 on each site

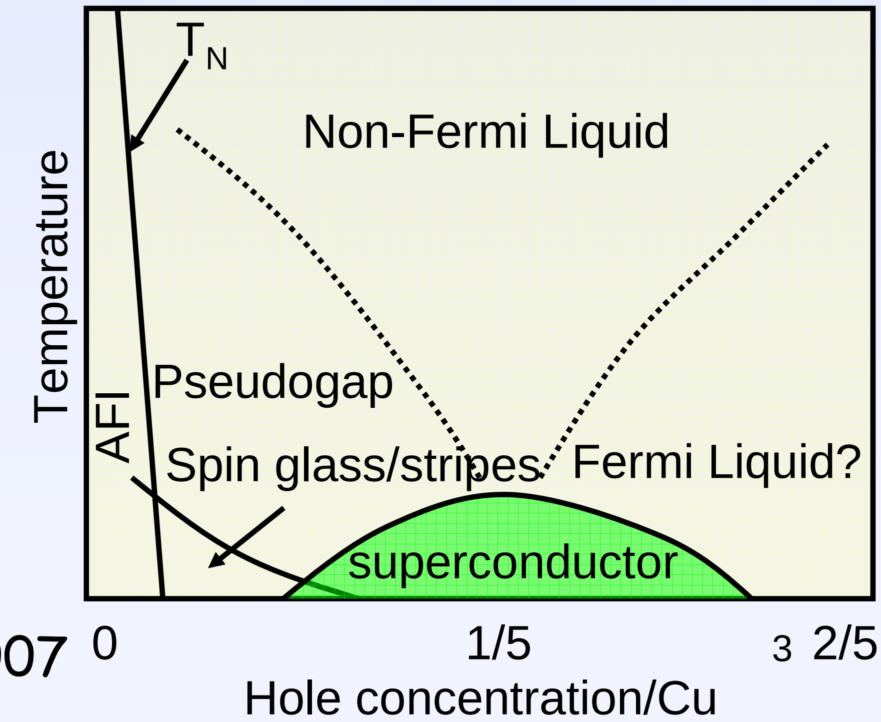




Single hole doping
Zhang and Rice PRB (1988)

$$\Psi_{ZRS}=(\phi(\alpha)d(\beta)-\phi(\beta)d(\alpha))$$





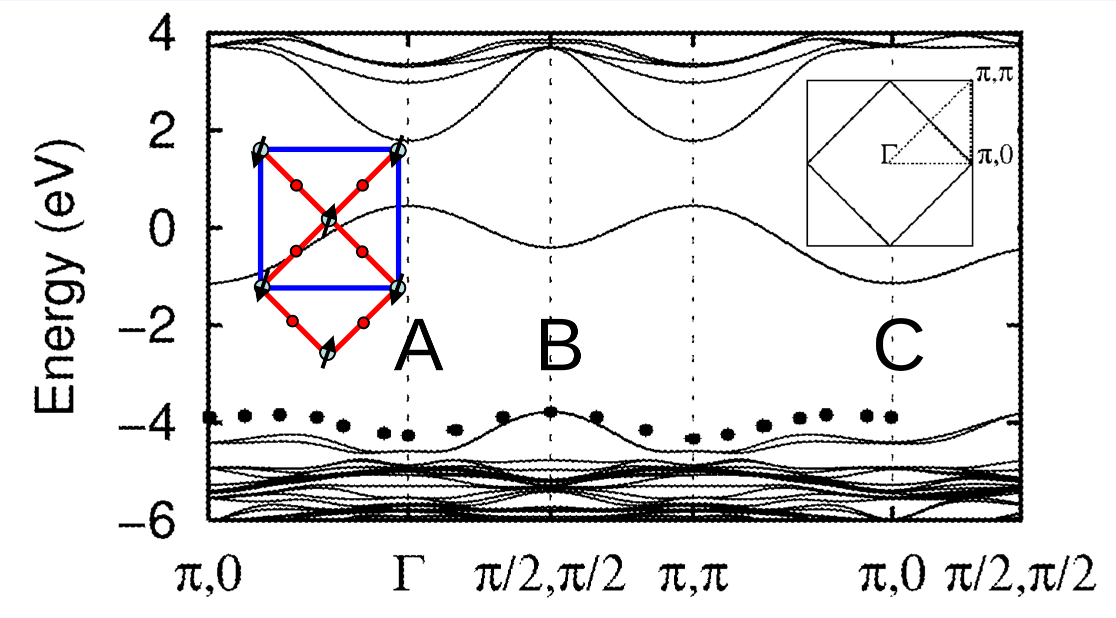
LCC 2007

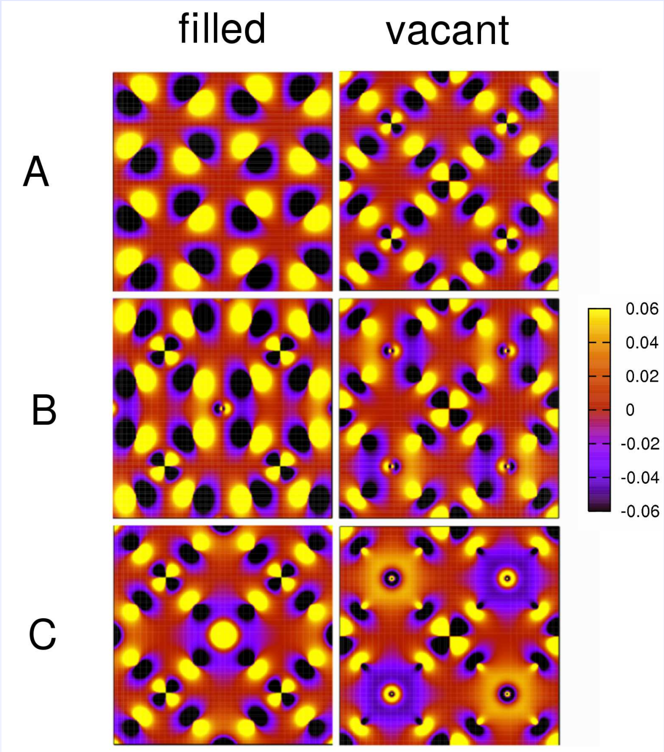
Hybrid DFT $Ca_2CuO_2Cl_2$

$$E_{xc} = (1-A)(E_x^{LDA} + BE_x^{Becke}) + AE_x^{HF} + (1-C)E_C^{VWN} + E_C^{LYP}$$

$$B3LYP: A = 0.2, B = 0.9, C = 0.81$$

Becke (1993), Stephens (1994)





Dots = t-J model
J/t = 0.4
t = 0.5 eV
Dagotto (1994)

Cuprate stripe history

Incommensurate Magnetic Fluctuations in $La_{2-x}Sr_xCuO_4$,
S. W. Cheong *et al.,* Phys. Rev. Lett. **67**, 1791-1794 (1991)

Incommensurate Magnetic Fluctuations in $La_{2-x}Sr_xNiO_4$,
S. M. Hayden *et al.,* Phys. Rev. Lett. **68**, 1061 (1992)

Evidence for stripe correlations of spins and holes in copper oxide superconductors
J. M. Tranquada, B. J. Sternlieb, J. D. Axe, Y. Nakamura, S. & Uchida, *Nature (London)* **375**, 561 (1995)

A 'checkerboard' electronic crystal state in lightly hole-doped $Ca_{2-x}NaxCuO_2Cl_2$,
T. Hanaguri *et al.,* Nature **430**, 1001 (2004).

Quantum magnetic excitations from stripes in copper oxide superconductors,
J. M. Tranquada *et al.,* Nature **429**, 534 (2004).

The structure of the high-energy spin excitations in a high-temperature superconductor,
S. M. Hayden, H. A. Mook, P. Dai, T. G. Perring and F. Dogan, Nature **429**, 531 (2004).

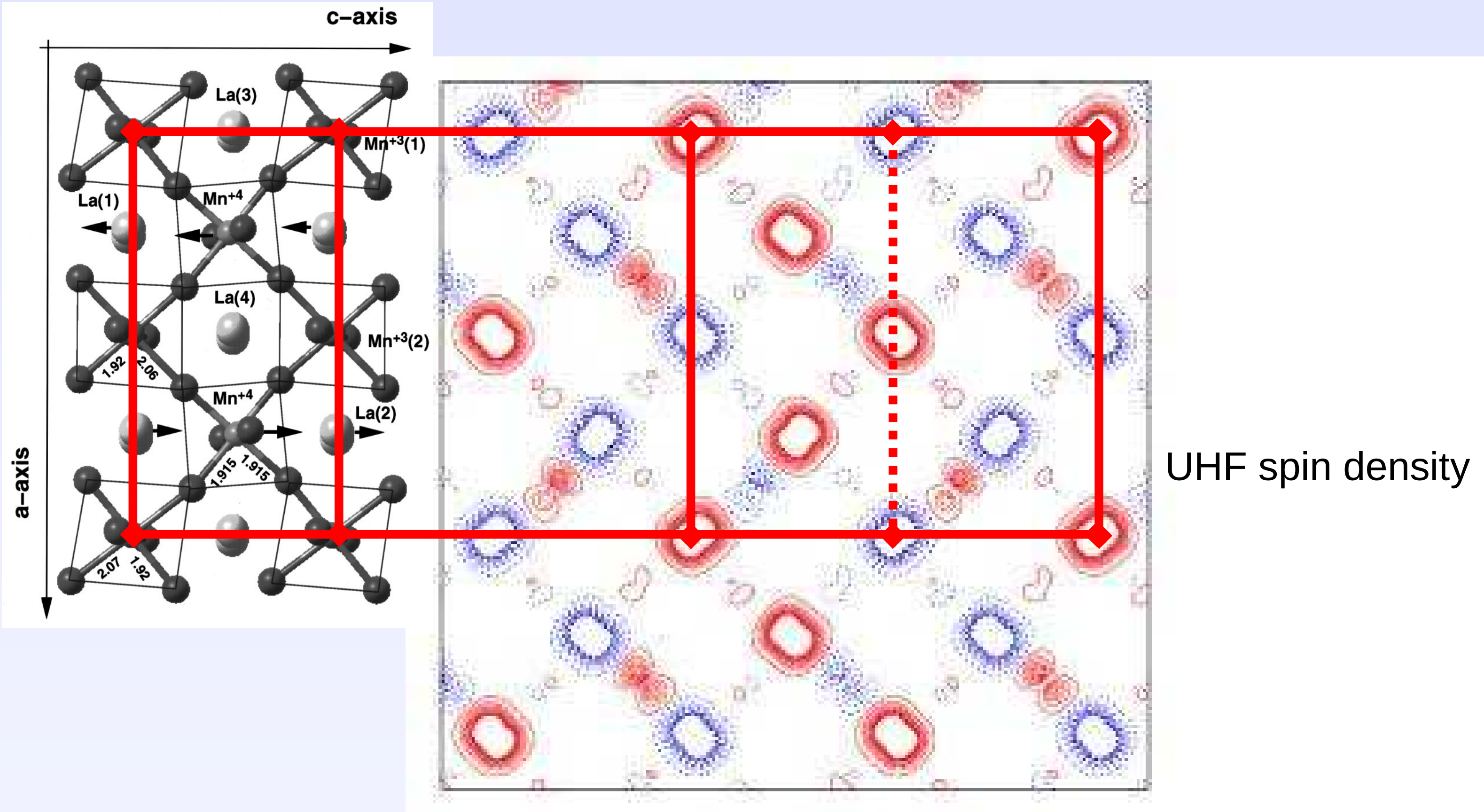
Computation of stripes in cuprates within the LDA + U method,
V. I. Anisimov *et al.,* Phys. Rev. B **70**, 172501 (2004).

Electron–phonon coupling reflecting dynamic charge inhomogeneity in copper oxide superconductors,
D. Reznik *et al.,* Nature, **440**, 1170 (2006).

An Intrinsic Bond-Centered Electronic Glass with Unidirectional Domains in Underdoped Cuprates,
Y. Kohsaka, *et al.,* Science **315**, 1380 (2007).

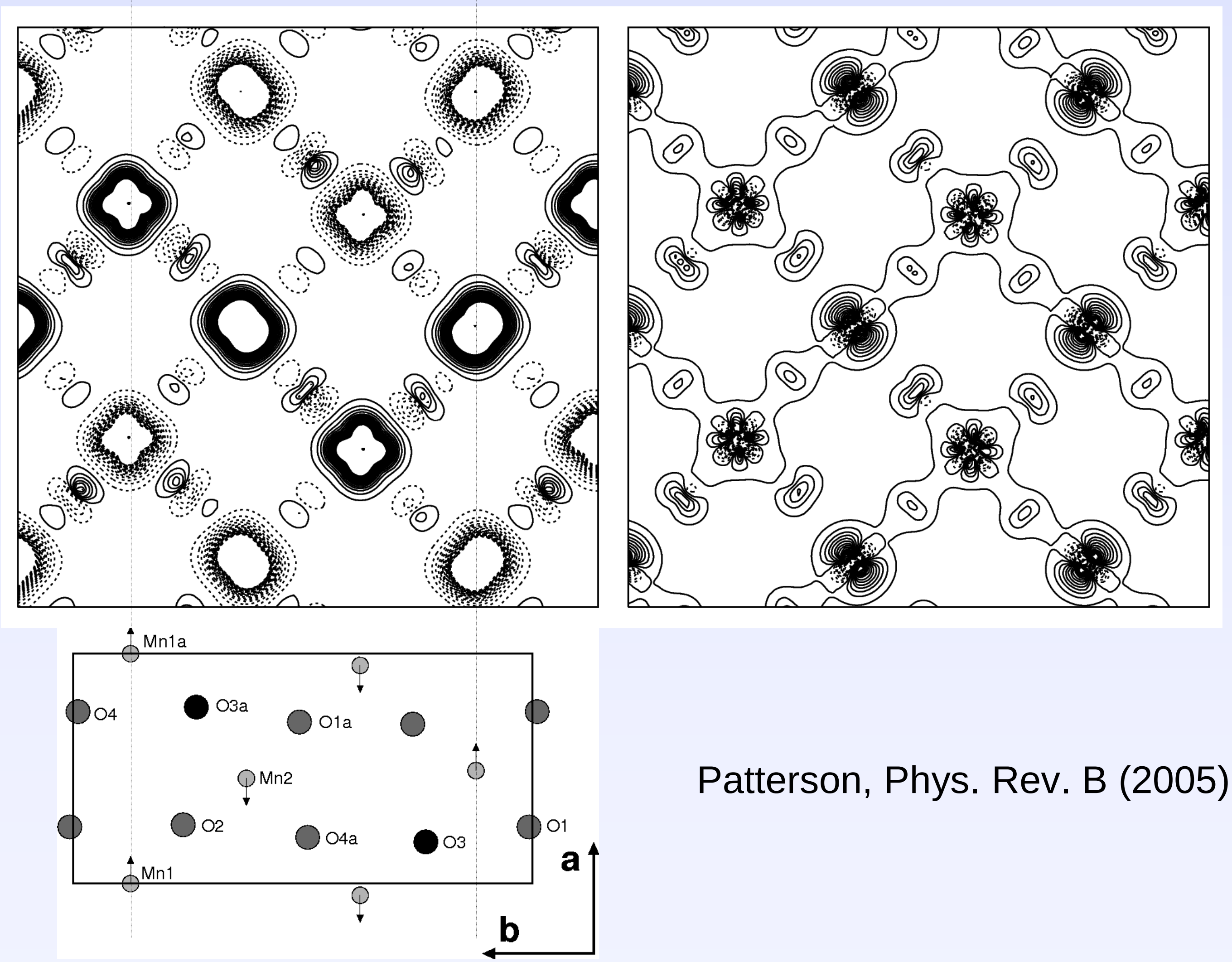
Angle-resolved photoemission studies of lattice polaron formation in the cuprate $Ca_2CuO_2Cl_2$,
K. M. Shen *et al.,* Phys. Rev. B **75**, 075115 (2007)

Zener Polaron Electronic Structure of $La_{1/2}Ca_{1/2}MnO_3$

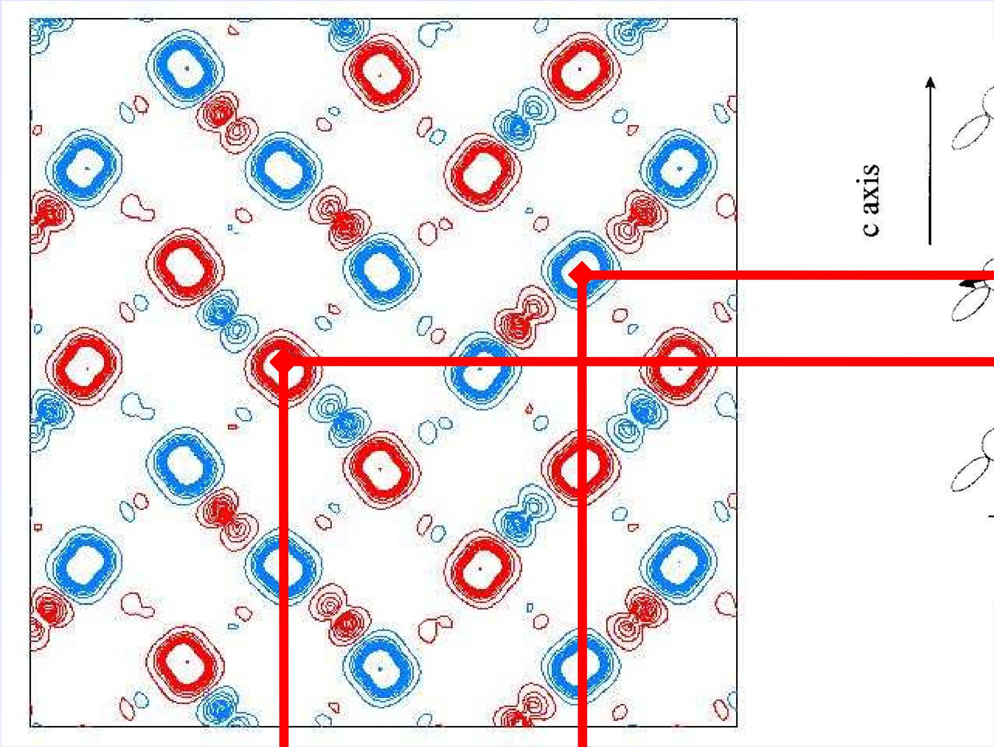


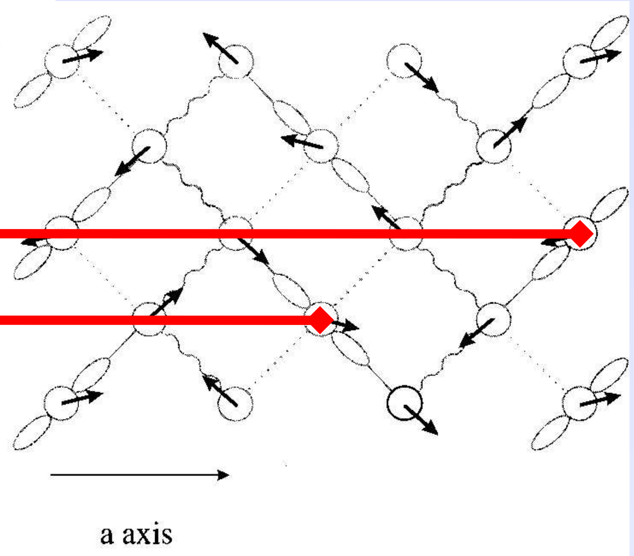
Zheng and Patterson, Phys. Rev. B (2003)

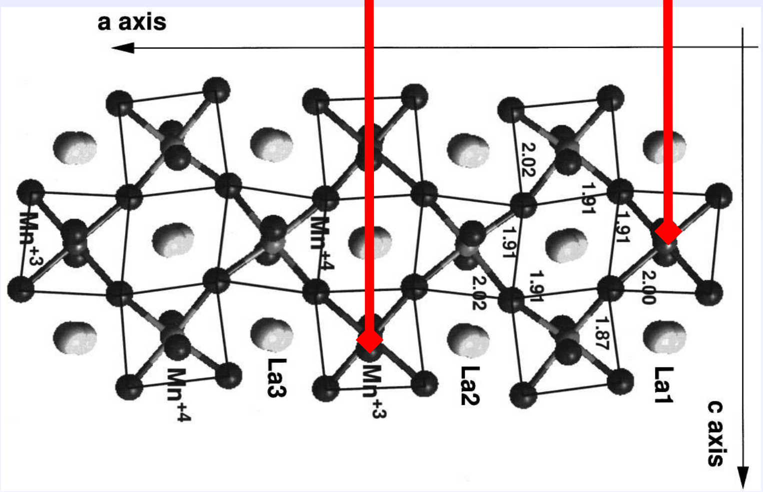
CE-type phase of $La_{1/2}Ca_{1/2}MnO_3$



Patterson, Phys. Rev. B (2005)





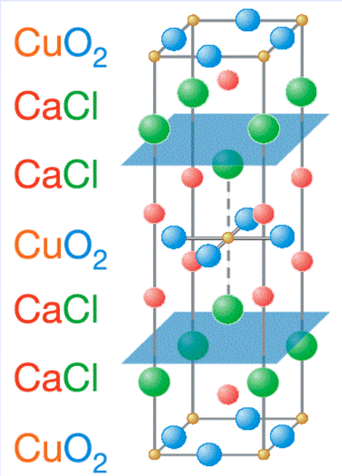


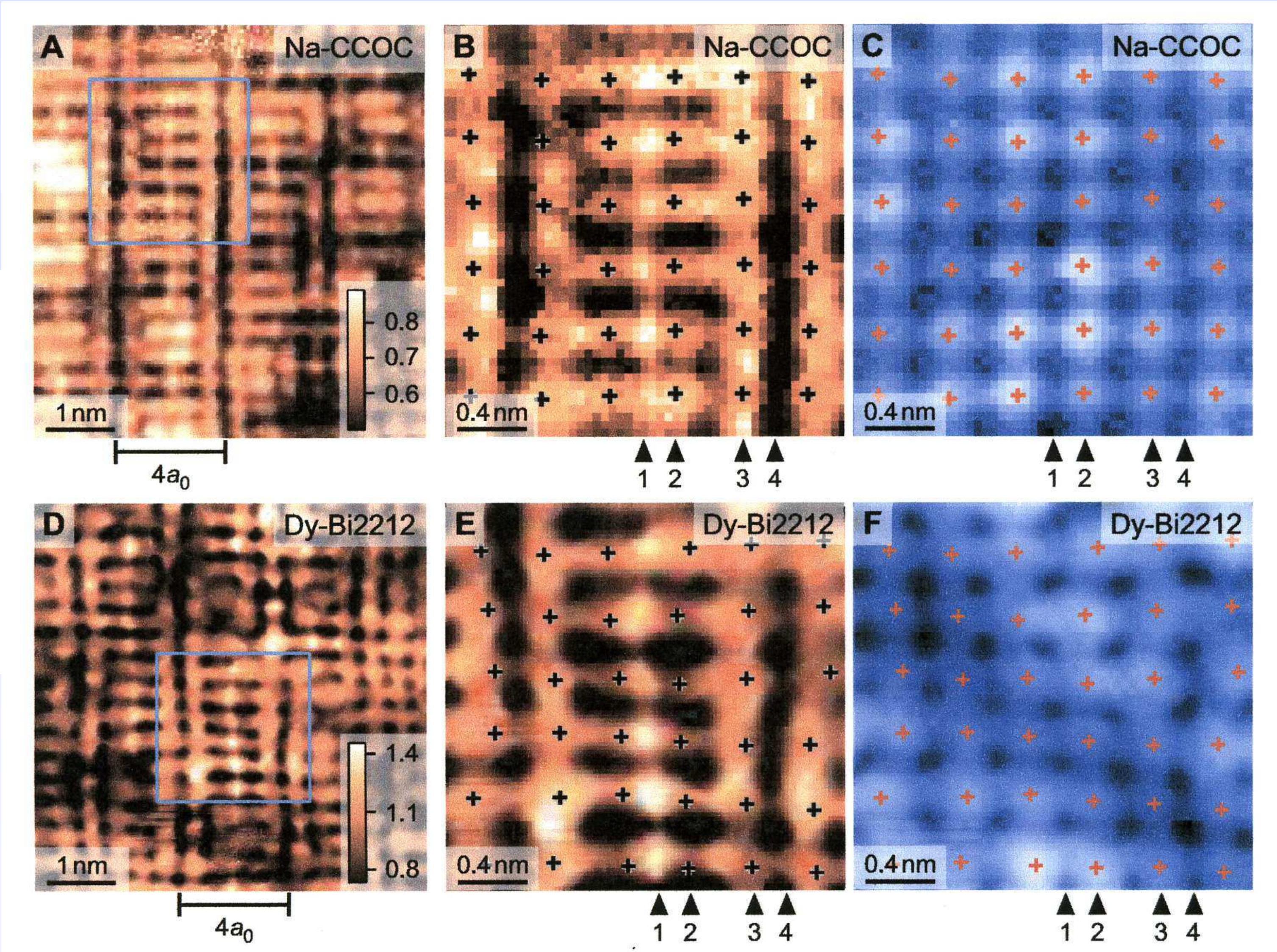
$La_{1/3}Ca_{2/3}MnO_3$ UHF spin density
CO on O ions not Mn ions!

Zheng and Patterson,
Phys. Rev. B (2003)

Neutron powder crystal structure
P. Radaelli *et al.*
Phys. Rev. B (1999)

1-D Stripes $Na_xCa_{2-x}CuO_2Cl_2$ x=1/8



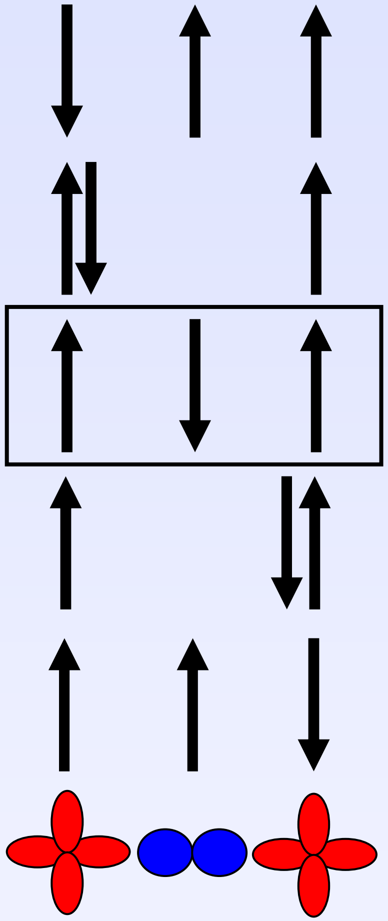


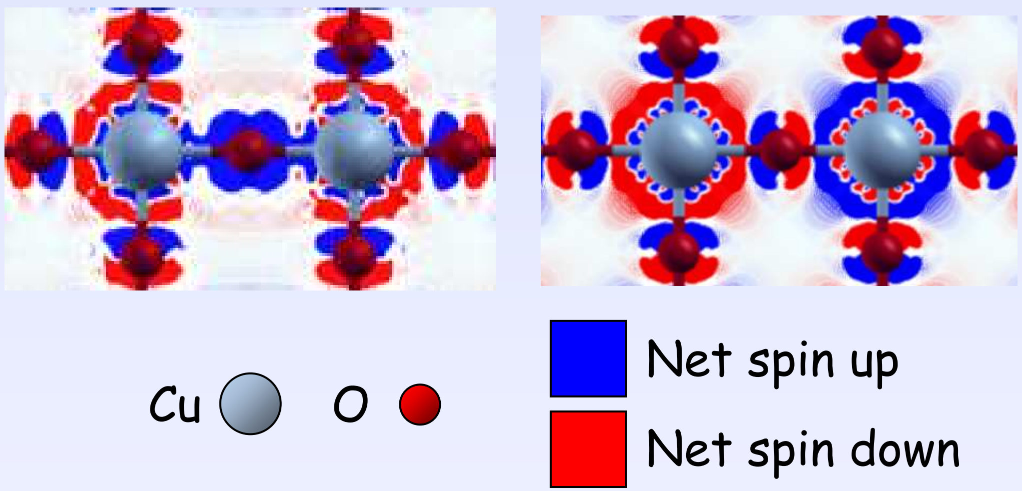
Y. Kohsaka et al. Science (2007)

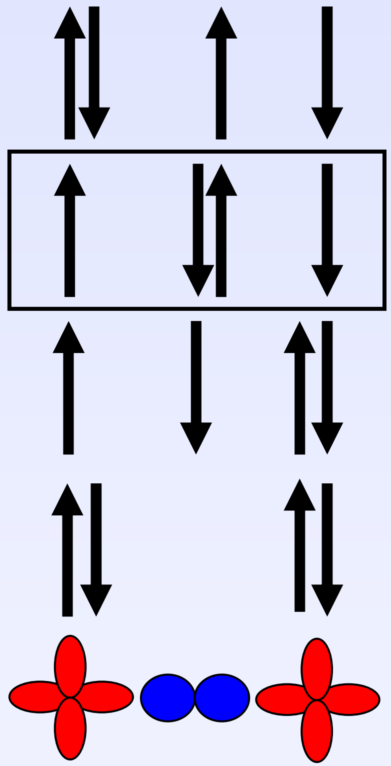
LCC 2007

O Cu Cu O

Double and Superexchange



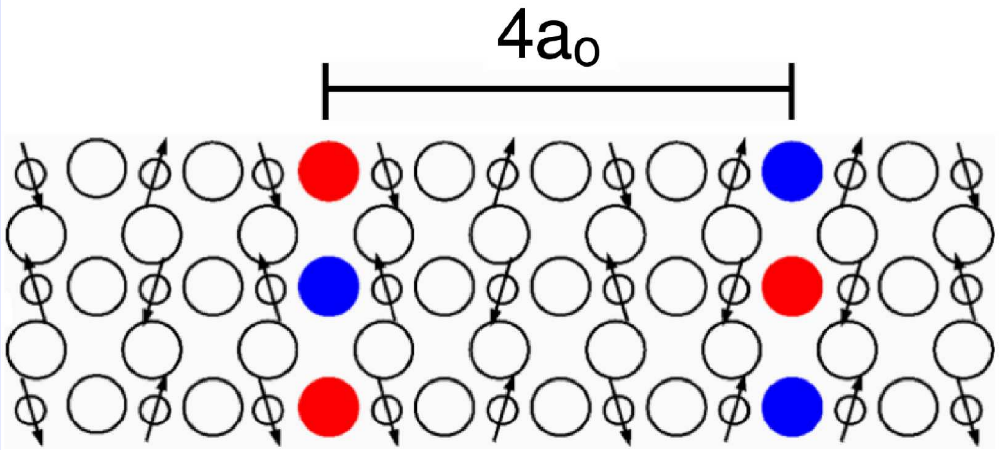




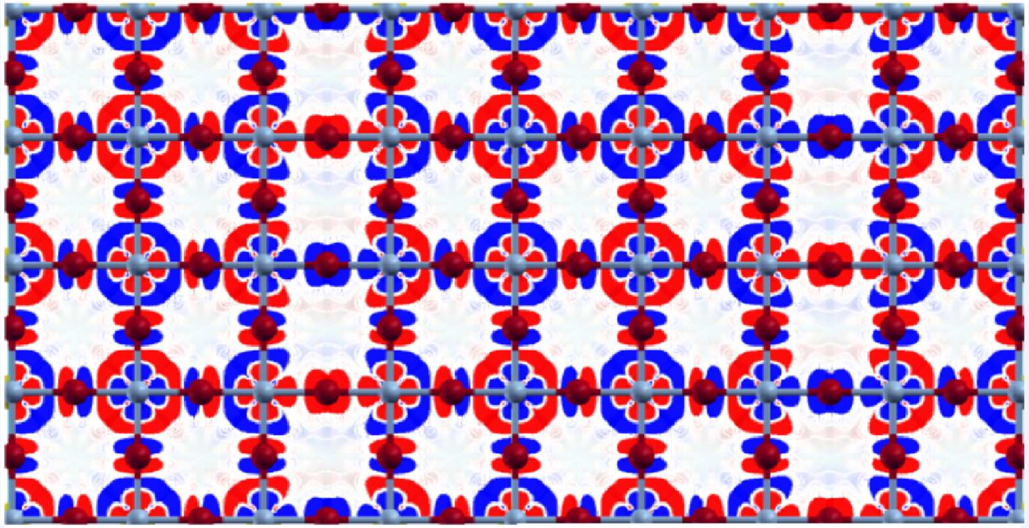
Double Exchange
Localised hole
Zener (1955)

Superexchange
No localised hole
Anderson (1969)

Hybrid DFT: $Na_xCa_{2-x}CuO_2Cl_2$ x=1/8

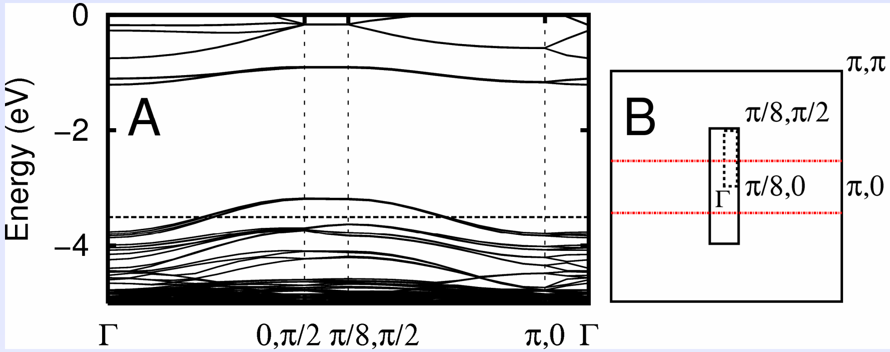


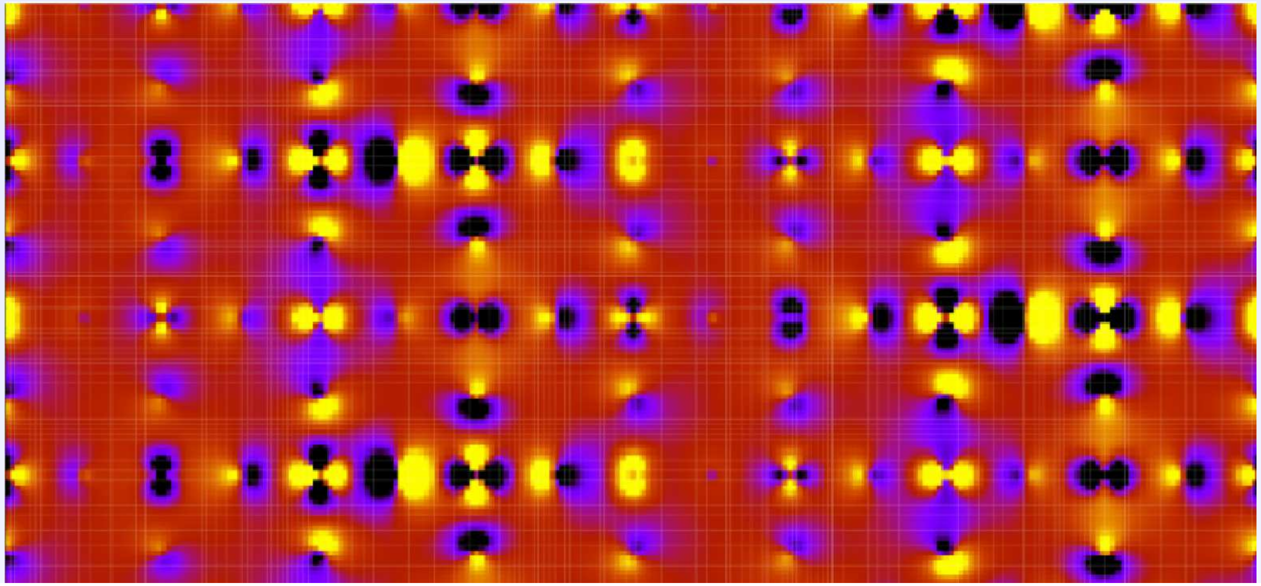
Magnetic Anti-Phase Boundaries



Spin Density

Hybrid DFT: $Na_xCa_{2-x}CuO_2Cl_2$ x=1/8

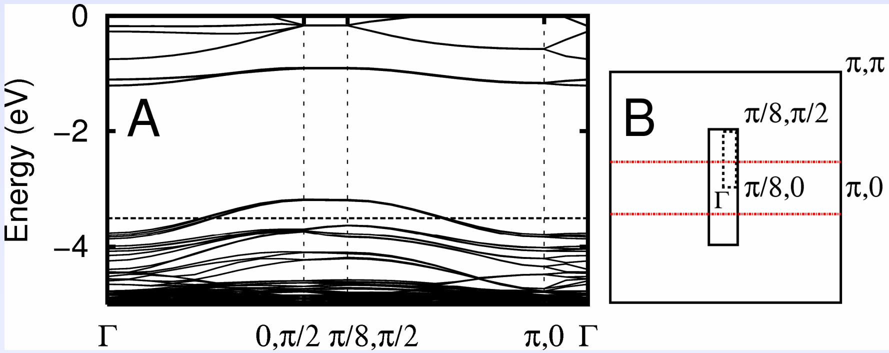




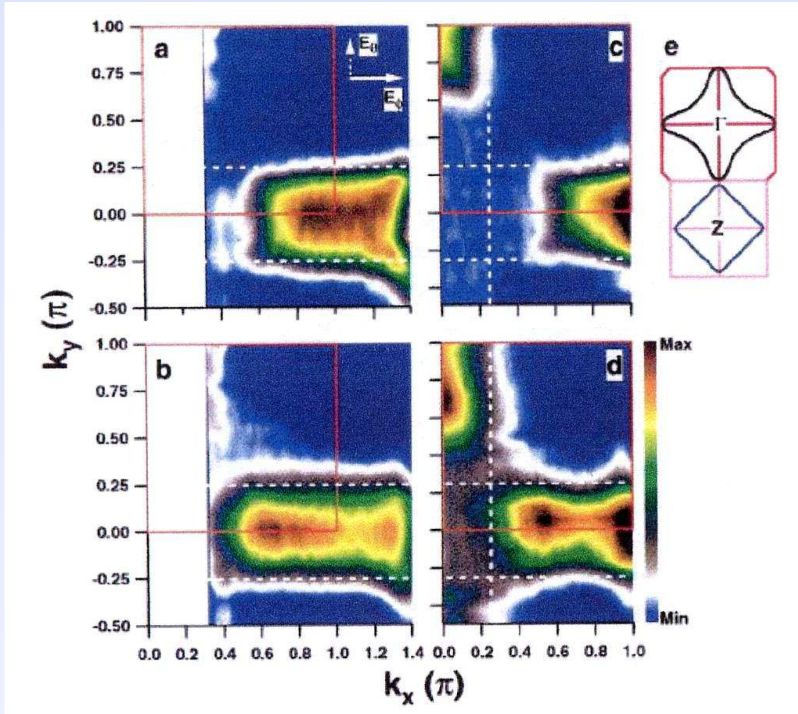
Stripe Band Wave Function Amplitude (Γ point)

Spectral weight of Nd-LCSO near ε_f

$Na_{0.12}Ca_{1.88}CuO_2Cl_2$



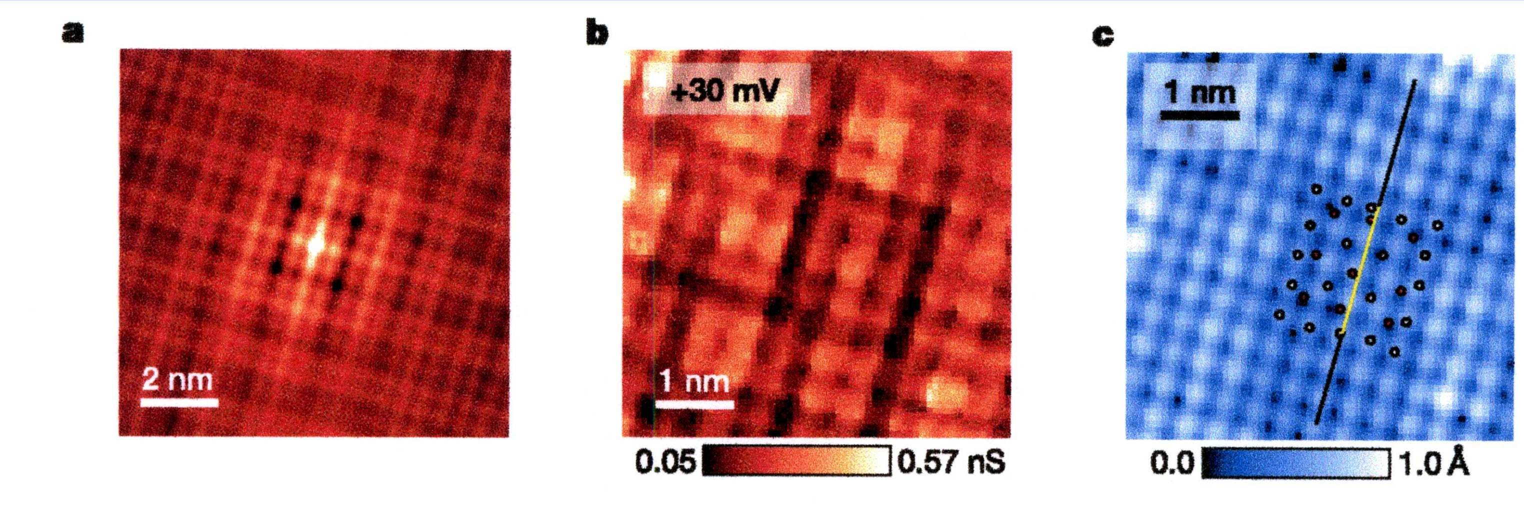
$(La_{2\text{-}x\text{-}y}Nd_ySr_x)CuO4$



Zhou et al. Phys. Rev. Lett. (2001)

(a) x=0.10, 30 meV
(b) x=0.10, 300 meV
(c) x=0.15, 30 meV
(d) x=0.15, 300 meV

4x4 'Tile' Phase in $Na_{0.1}Ca_{1.9}CuO_2Cl_2$



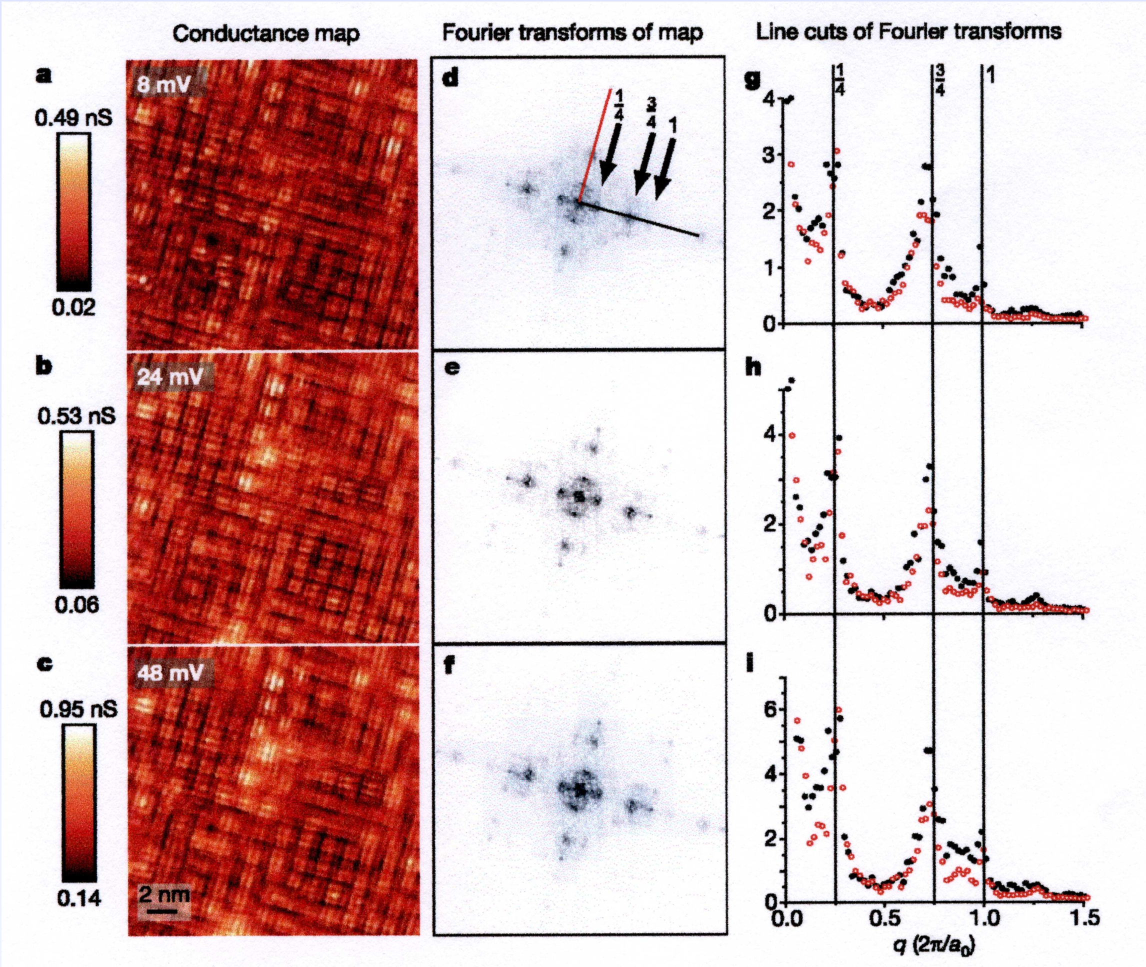
autocorrelation

dI/dv
conductance α PDOS

topographic

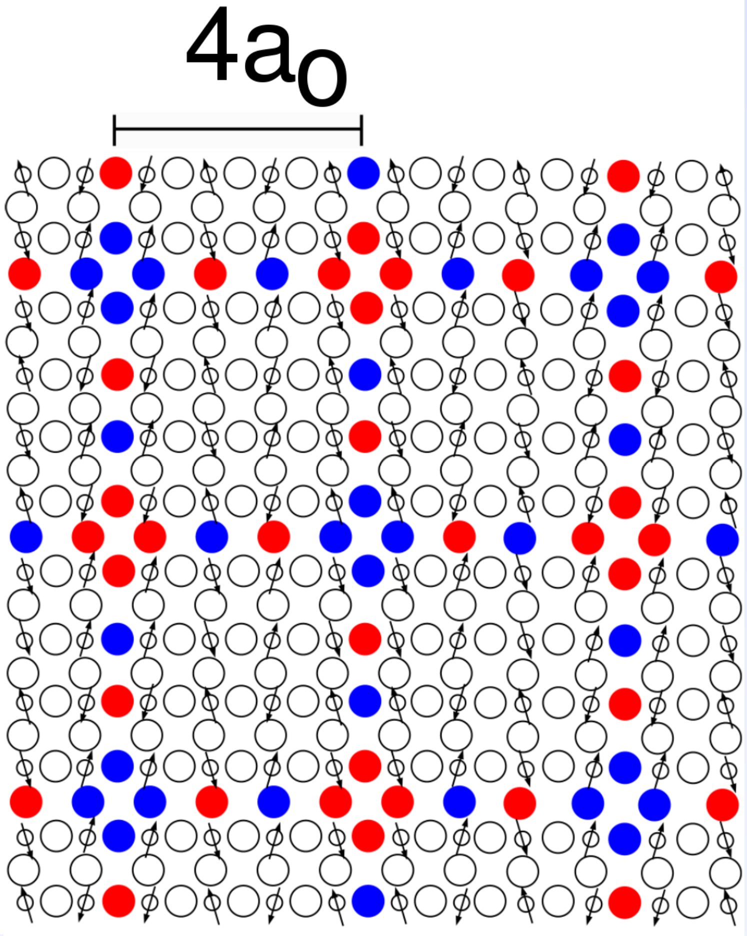
Hanaguri *et al.* Nature (2004)

4x4 'Tile' Phase in $Na_{0.1}Ca_{1.9}CuO_2Cl_2$

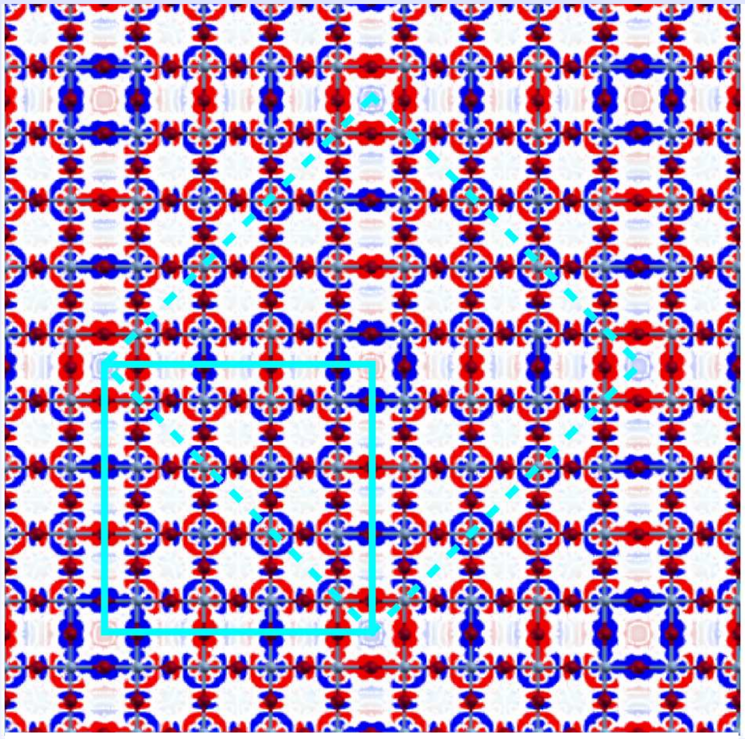


Hanaguri *et al.* Nature (2004)

Hybrid DFT: $Na_xCa_{2-x}CuO_2Cl_2$ x=1/8

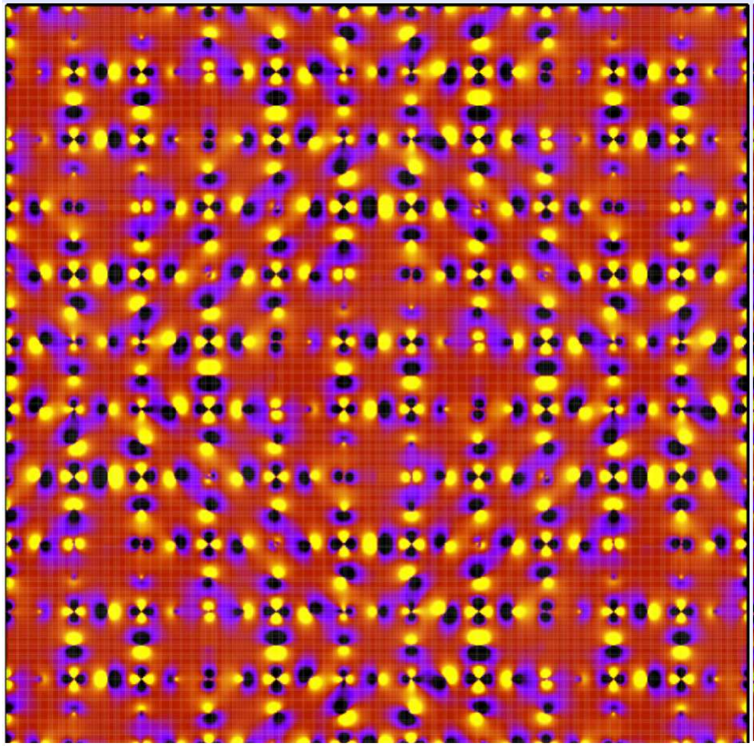


Magnetic Anti-Phase Boundaries

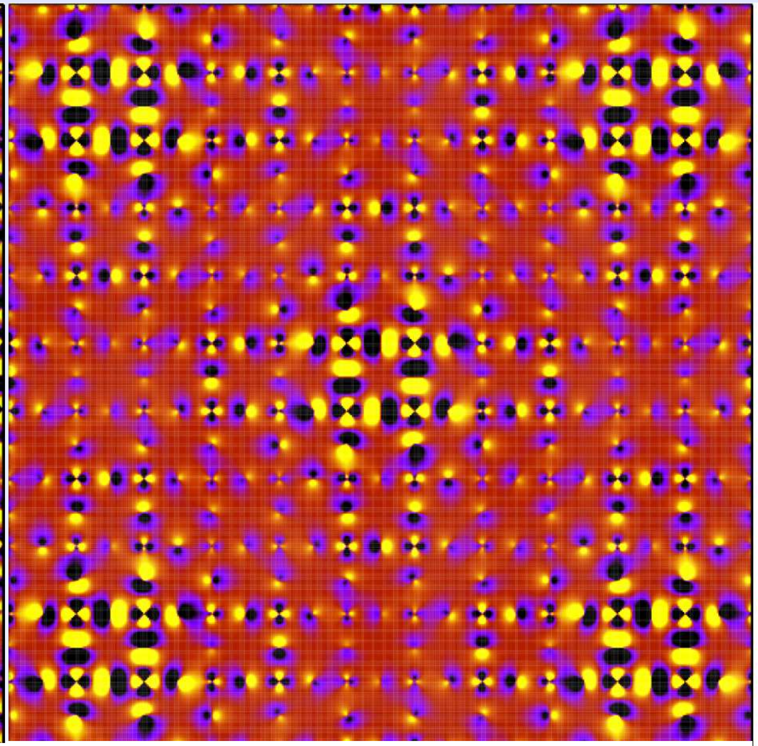


Spin Density

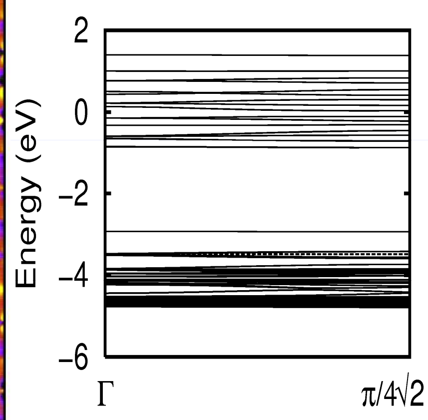
Hybrid DFT: $Na_xCa_{2-x}CuO_2Cl_2$ x=1/8



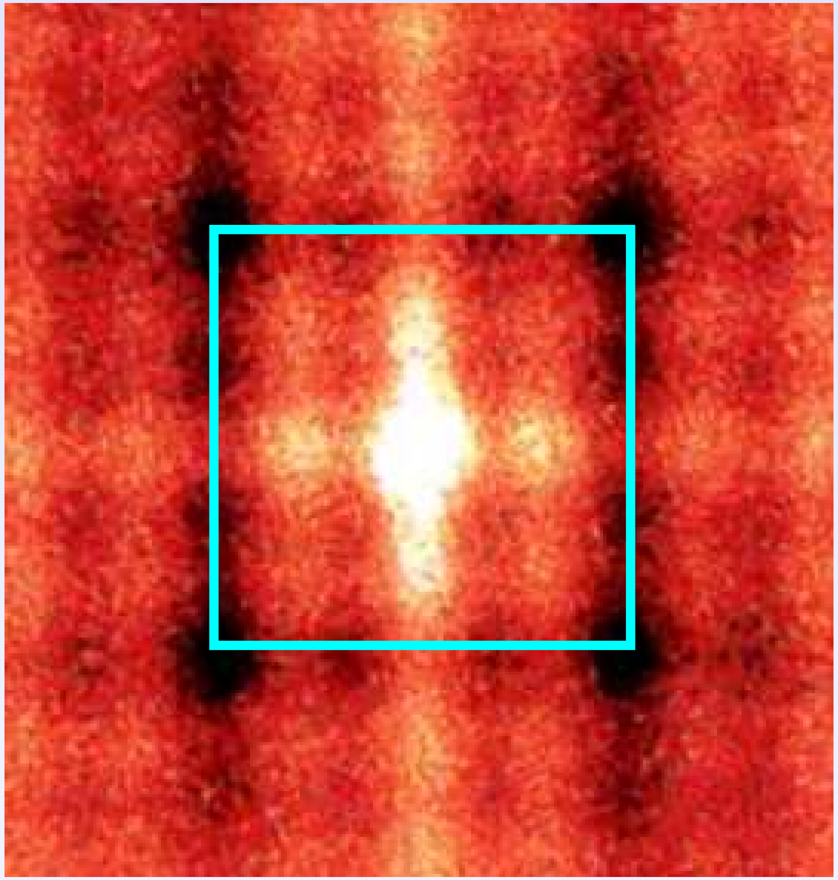
Ψ Amplitude (Γ point, occupied)

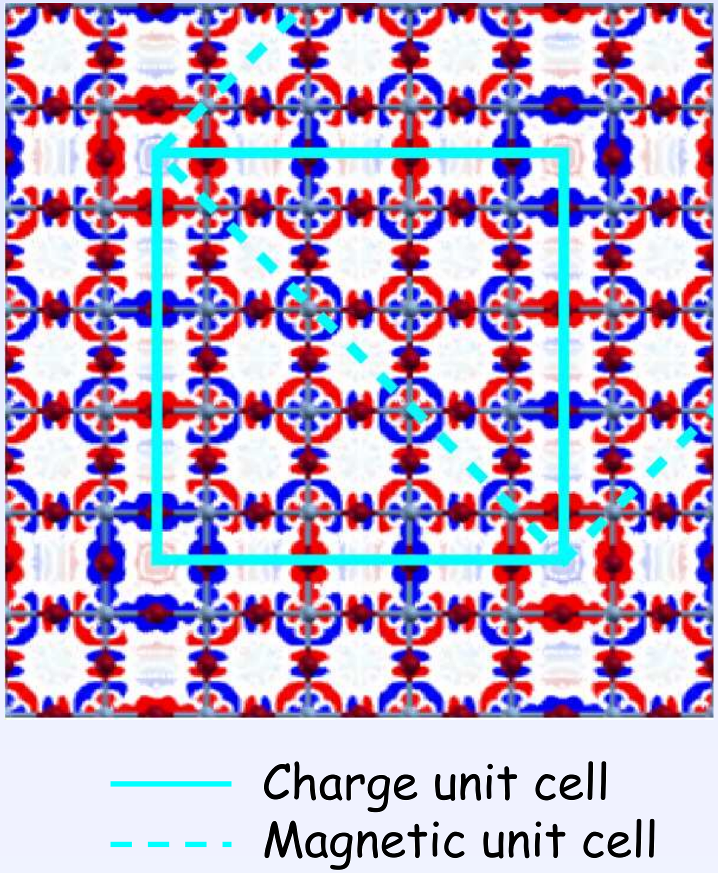


ΨAmplitude (Γ point, band gap)

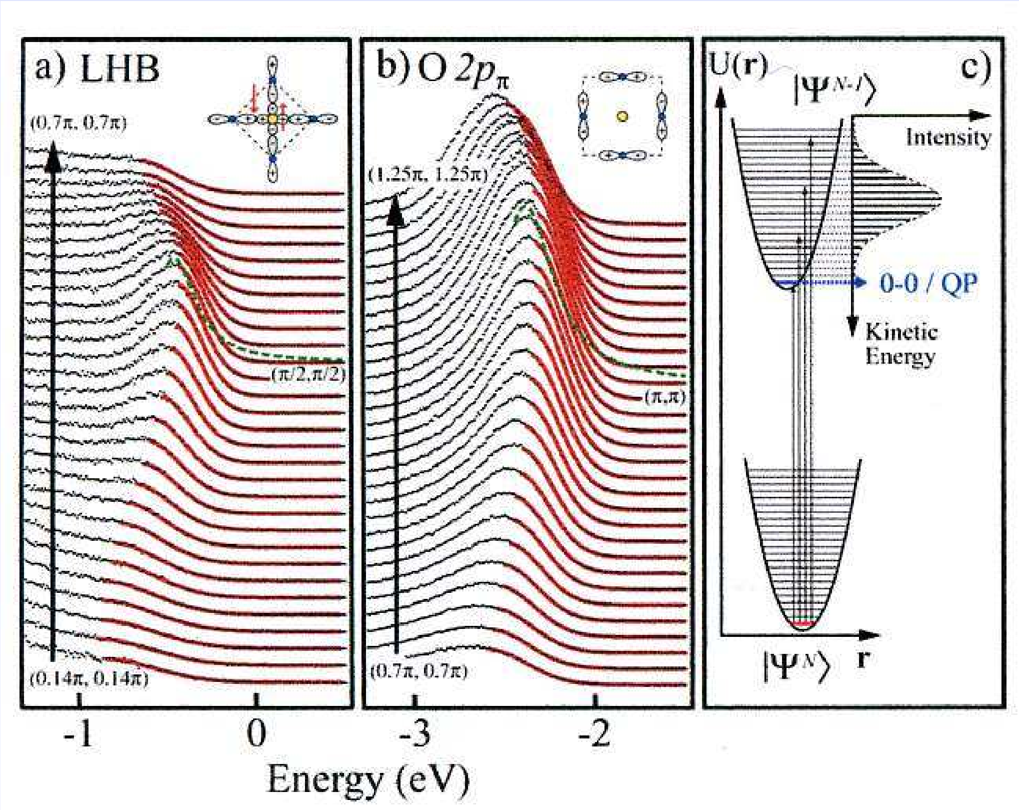


4√2x4√2 Magnetic Supercell





Recent Photoemission $Ca_2CuO_2Cl_2$



Photoemission lineshapes well fitted by Gaussian profile
Both LHB and O 2pπ states broadened into Gaussian
Broadening mechanism is phonon, not magnon
Photo-holes are small polarons

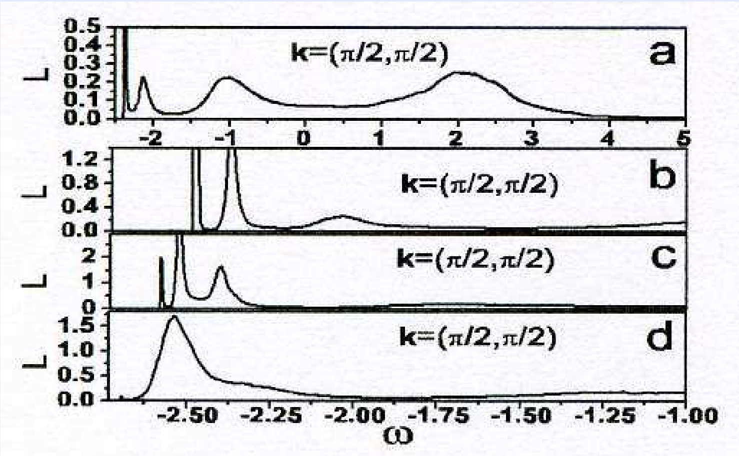
LCC 2007 Shen et al. PRB 2007

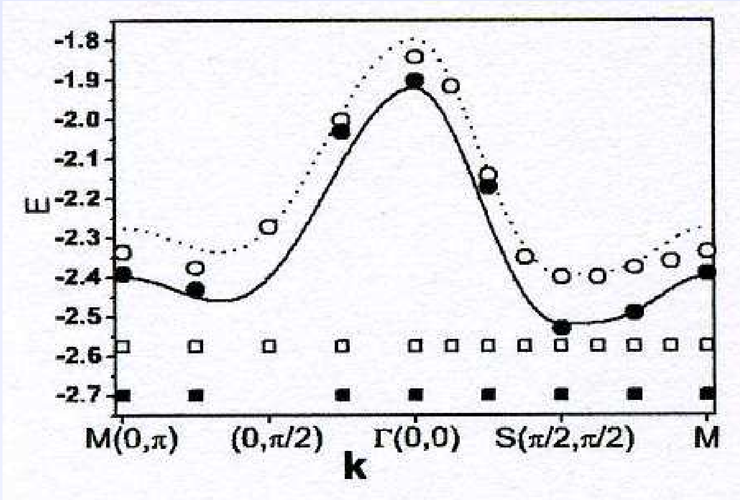
t-J + electron-phonon coupling

$$H = H^{t-J} + H^{e-ph}$$

$$H^{e-ph} = \Omega \sum_k b_k^+ b_k + \frac{\gamma}{N} \sum_{k,q} \left[h_k^+ h_{k-q} b_k + H.c. \right]$$

$$g = \frac{\gamma^2}{8t\Omega}$$



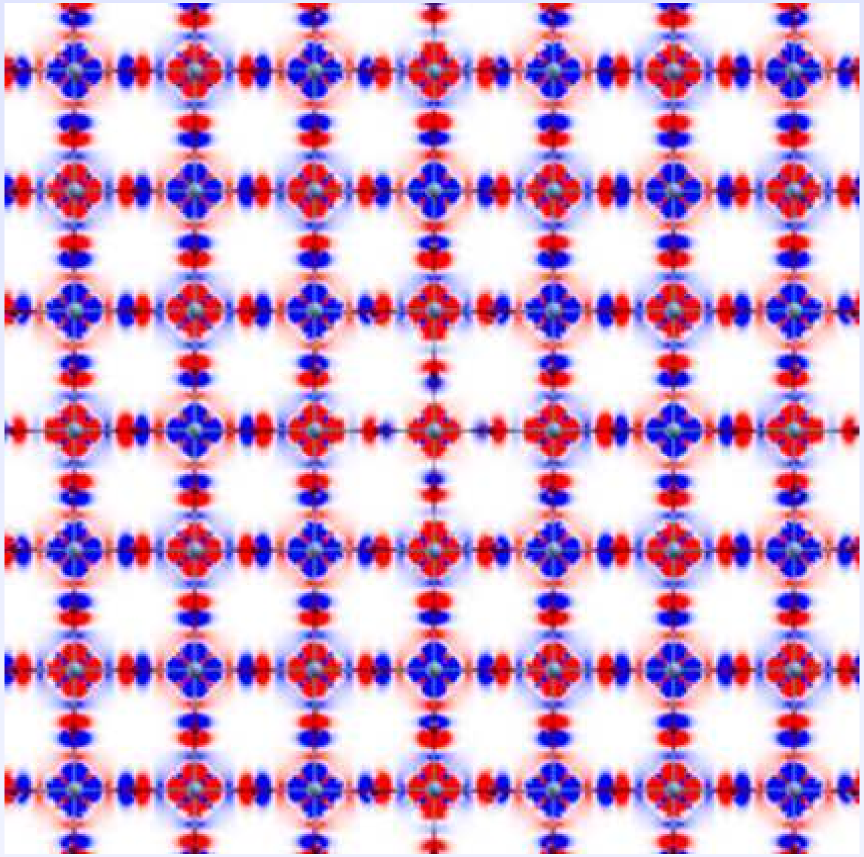


(a) g = 0
(b) g = 0.14 γ = 0.34
(c) g = 0.20 γ = 0.40
(d) g = 0.23 γ = 0.43

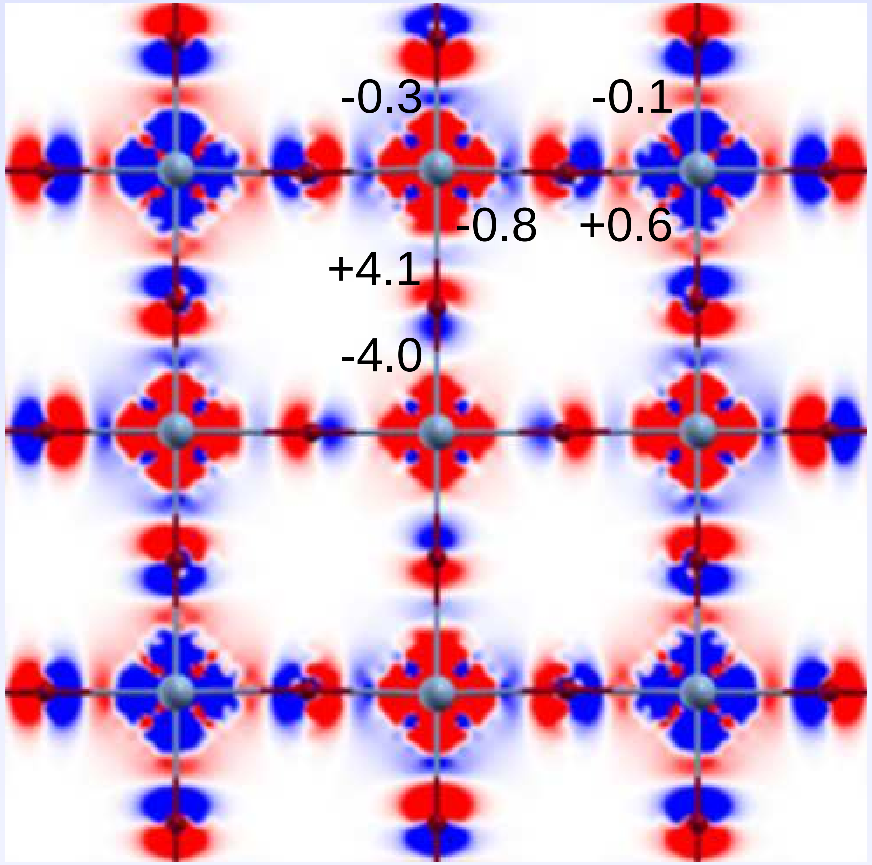
Spectral function consists of self-trapped quasi-particle state with vanishing spectral weight plus 'broad feature' which tracks t-J dispersion

Mischenko and Nagaosa, PRL 2004

Small polarons: $Na_xCa_{2-x}CuO_2Cl_2$ x=1/32

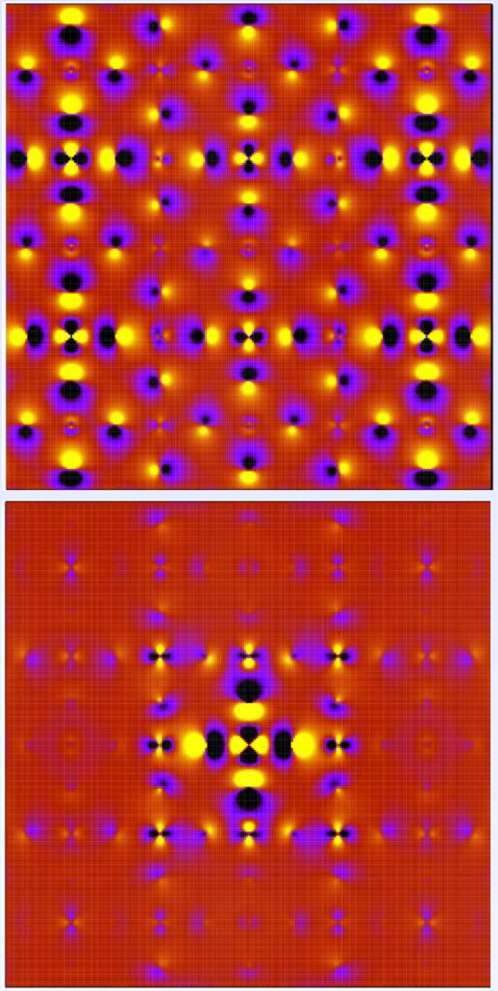


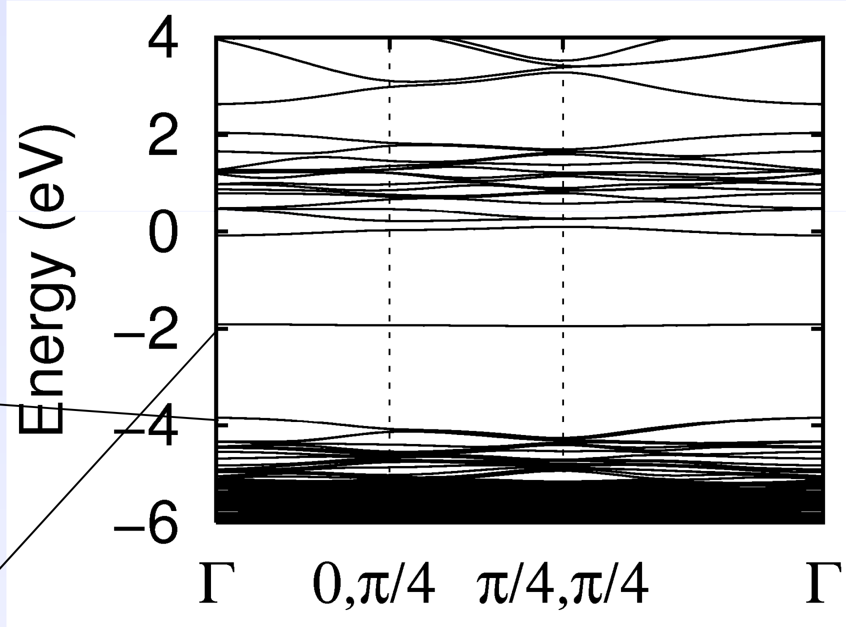
Bond length changes (%)



B3LYP A = 0.3

Small polaron band structure





Polaron band structure

Calculation performed in 4x4 cell
Hole localises for A = 0.3
Vacant state formed at mid-gap

Conclusions

- Polarons key to understanding doped oxides
- Local charge order on O ions
- How do stripes/polarons affect Tc in CMR, HTS, DMS oxides?
- Hybrid DFT
  – short range properties need more exchange
  – Long range properties need less exchange

Acknowledgements

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