Functional Complexity in Soft Electronic Matter

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With: K. Ahn, A. Balatsky, A. Bussmann-Holder, G. Kalosakos, E. Kaneshita,
I. Martin, J. Phillips, C. Reichhardt, C.J.Olson-Reichhardt, A. Saxena,
S. Shenoy, T. Lookman, N. Voulgarakis, J-X Zhu

- New generations of experimental precision are driving new multiscale modeling / frameworks for many "strongly correlated" electronic materials (inorganic, organic, biological)

- An era to accept, understand, and exploit "intrinsic complexity"

From "The Physics of Materials, How Science Improves our Lives"

National Academy Press, 1999

- "…. today our challenge is to extend that understanding to more **complex** forms of matter - and to more complex phenomena … **a whole new style of inquiry** …"

- "It is becoming increasingly **interdisciplinary**, with progress often being made at the interfaces of biology, chemistry, materials science, and atomic and molecular physics."

- "A community more closely connected with industry and with the rest of science and **armed with experimental and computational capabilities that were not even imaged just a few decades ago."**

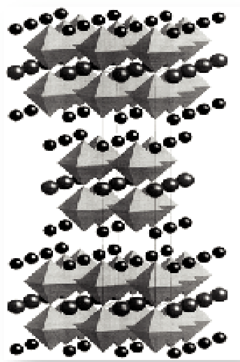
"Systems Biology"

http://www.icsb2001.org/what_is.html

The goal of Systems Biology is the construction and experimental validation of models that explain and predict the behavior of biological systems…. Characterized by a synergistic **integration of theory, computation, and experiment.** Only through this inter-disciplinary approach can we achieve a multiscale, multiresolution understanding of complex biological processes.

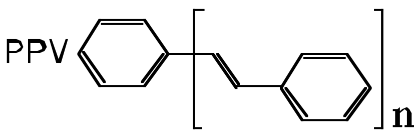
Examples of Functional, Multiscale Complexity in "Soft Matter"

* **Transition metal oxides (HTC, CMR, FE…)**



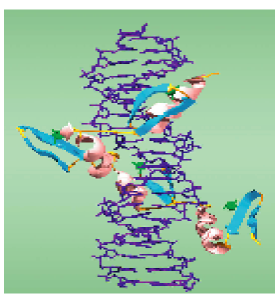
e.g.,
Nature **428,**
401 ('04)
Euro Phys. Lett. **71**,
249 ('05)

* **Conjugated organic polymers**



e.g.,
PNAS **100,**
2185 ('03)
Nature ('06)

* **Biological macro-molecules**



- **Myoglobin**
- **DNA**
  e.g.,
  Nucl. Acids. Res. **32,** 1589 ('04)
  Phys Rev. Lett. ('06)
- **Rafts**

Coupled
Spin-Charge-Lattice
(Strain)

Strongly correlated,
intrinsically
soft, multiscale, glassy;

Correlated "Hotspots" ;

Adaptive intermediate phases
- functioning at the "nonhomogeneous edge"
(PRL 94, 208701 ('05))

Systems/Networks of connected, functional scales (structural <u>and</u> electronic)

- Long-range consequences of local constraints
- Coexisting short- and long-range interactions

Electrostatics:
Bundling of Like Charged Objects

Long Range Interactions
Ernshaw: Coulomb systems are unstable

Short Range Repulsion
Define Geometry: Prevent Coulomb collapse

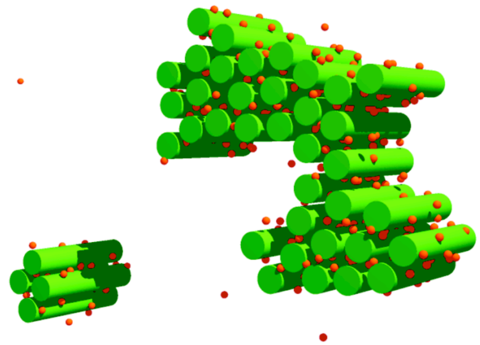
Entropy
Thermal Effective Repulsion

→ Marginal Balance between Repulsion and Attraction Provides for Sensitive Macroscopic Manipulation

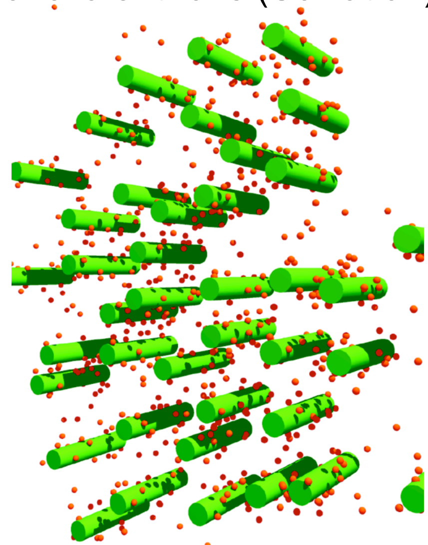
Model System Example:
Like Charged Rods (Polyelectrolyte)
Point Counter Charge (Salt)
Thermal Noise (Room Temperature)

→ Nanotribology/adhesion
Polyelectrolyte self-assembly
Gels, Colloids, Membranes
Macromolecular aggregation

Divalent Ions (Aggregation)



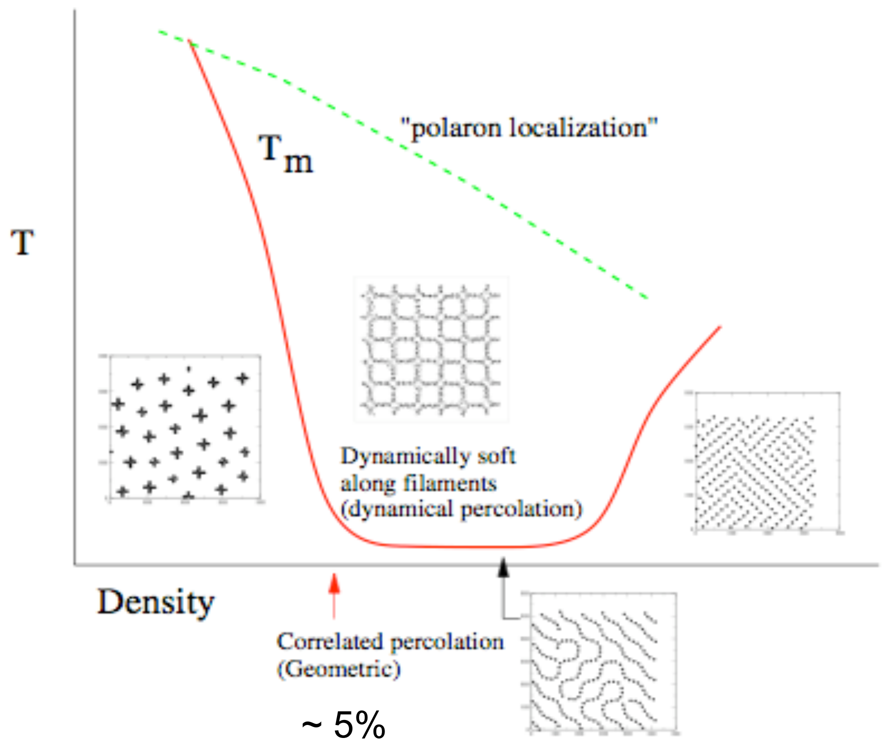
Monovalent Ions (Solvation)



Jensen et.al., *PRL* **78,** 2477 ('97)

Fibrillar templates and soft phases in systems with short-range dipolar and long-range interactions

Stojkovic et al., *PRL* (‘99); Reichhardt et al., *PRL* **92**, 016801 (‘04)



cf. Isotropic short & long *PRL* **90**, 026401 (‘03); *Europhys. Lett.* **61**, 221 (‘03)

c.f. Gor’kov, Mueller, Emery/Kivelson… : Phase separation/coexistence

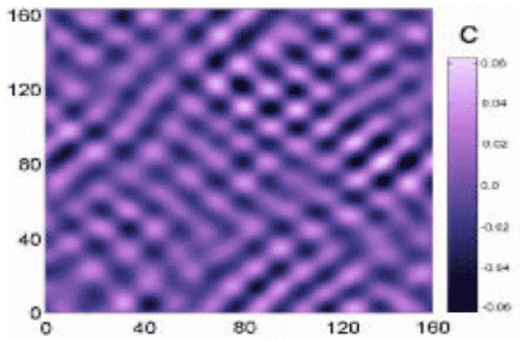
cf. Phillips (*PRL* **88**, 21640 (‘02)) : Spinodals

cf. Davis…. : STM “checker-boards”

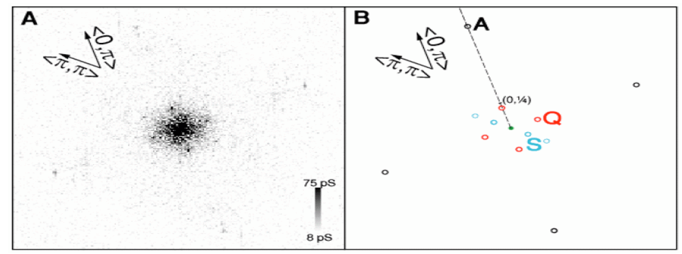
cf. Mihailovic et al. (*PRL*(‘05)) : Polarons

STS Imaging of HTC Cuprates

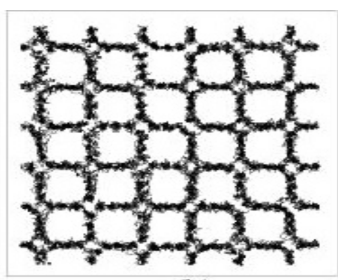
Checkerboard (Tweed) Stripes



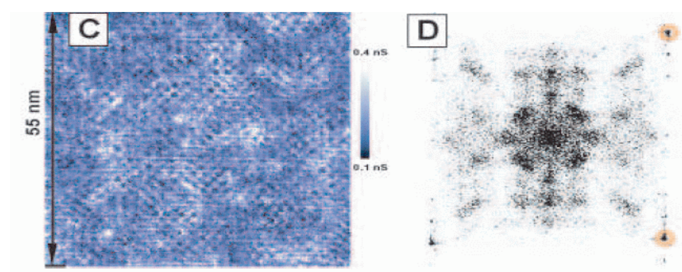
C. Howard et al., *PRB* **67,** 014533 (‘03)



A. Vershinin et al., *Science Express* (2/11/04)



(<u>Simulated</u>) C.J.O. Reichhardt et al., *PRL* **92**, 016801 (‘04)
Dipolar Forces



K. McElroy et al., cond-mat/0404005
Nature **430,** 1001 (‘04)

High Sensitivities of Transition Metal Oxides to Pressure/Strain

e.g.,

"Shape-Memory AF"

!

e.g.,

"Colossal Stresso-Resistance"

!

↓

Significant Cross-correlated Sensitivities

- **HTC Cuprates**

  e.g., Tritt et al., *PRL* **68**, 2531 (1992)
  Sarrao et al., *PRB* **50,** 13125 (1994)
  Gao et al., *PRB* **50,** 4260 (1994)
  Sato and Naito, *Physica C* **274,** 221 (1997)
  Nakamura et al., *PRB* **61**, 107 (2000)
  Lavrov et al., *Nature* **418,** 385 (2002)
  Bozovik et al., *PRL* **89,** 107001 (2002); *Nature* **421** (2003)
  Pavuna et al., *PRL* 057002 (2003)
  Oyanagi et al., (2006)

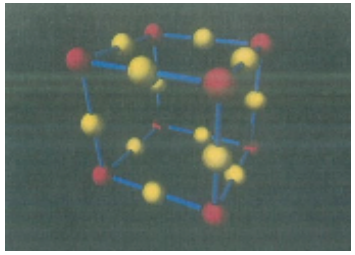
- **CMR Manganites**

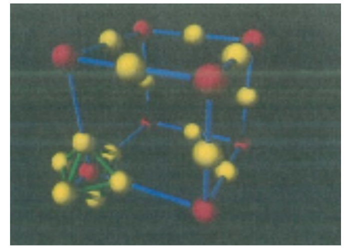
  e.g., Hwang et al., *PRB* **52**, 15046 (1995)
  Biswas, et al., *PRB* 63, 184424 (2001)
  Mathur et al., *Nature* **387**, 266 (1997)
  Renner et al., *Nature* **416,** 518 (2002)
  Wu et al., *Nature* (2006)

- **Ferroelectrics**

  e.g., Roth et al., *Ferroelectrics* **74,** 331 (1987)
  Wang et al., *PRB* **62**, R3577 (2000)

Athermal Local Structure in Perovskite Oxides
(HTC, CMR, FE, LAVES…)

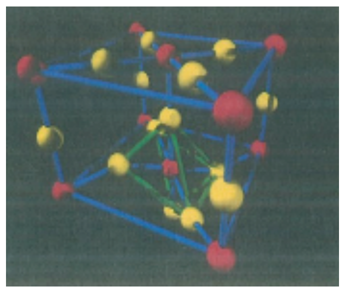


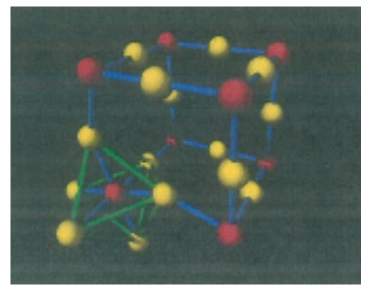


Directional bonding (d, f ….)

XAFS, PDF, STM, EPR …   Intra-cell (low-symmetry) distortions (e.g. polaronic)

c.f. *ab initio* electronic structure (supercells) e.g.
B. Klein *PRL* (1997);
O.K. Andersen *PRL* (2002) …





Lookman et al.,
PRB **60,** R12537 ('99);
67, 24114 ('03)

ORIGINS: Local bonding CONSTRAINTS [→ short-range + long-range(anisotropic strain)]
⊕ "Proximity" (T, P, M, doping…) to FIRST-ORDER P.T. (solid-solid)

CONSEQUENCES: ENTROPY-driven P.T; Extended precursor regimes (T, P, M, doping ….)
"Giant" precursor effects (Structural, Electronic; Elasticity, Polarization)
- Coexistence Landscapes; Filamentary; Correlated Percolation…
- Global ⟷ Local sensitivity

SOLID-SOLID PHASE TRANSFORMATION

Elasticity and Compatibility on a Triangular Lattice

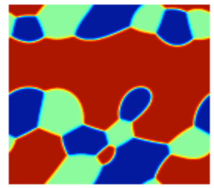
Lookman et al., ('01)

$$F = A e_1^2 + T(e_2^2 + e_3^2) - \frac{1}{3}(e_2^2 - 3e_2 e_3^2) + \frac{1}{4}(e_2^2 + e_3^2)^2 + \frac{1}{2}\left[(\nabla e_2)^2 + (\nabla e_3)^2\right]$$

bulk modulus (→ A)

Theory

$A = 0$



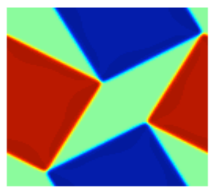
No Compatibility

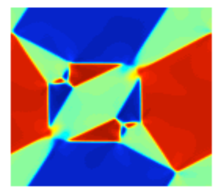
e_1 **Compression**

e_2 **Deviatoric**

e_3 **Shear**

$A = 22$

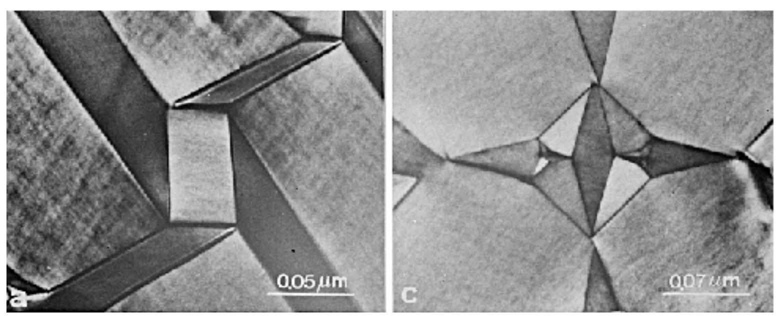




$A = 222$

With Compatibility

Experiment



Lead Orthovanadate

Amelinickx and van Tendeloo '86 (HREM)

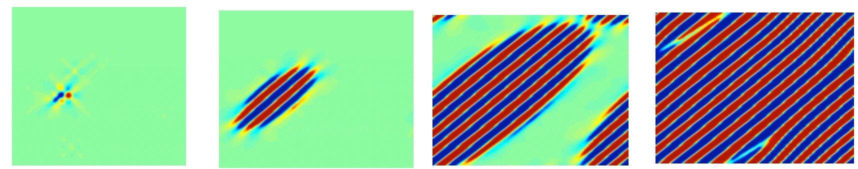
SIMULATION OF GINZBURG-LANDAU WITH COMPATIBILITY CONSTRAINTS

[Lookman et al., *PRB* **60**, R12537 (‘99); **67,** 2414 (‘03)]

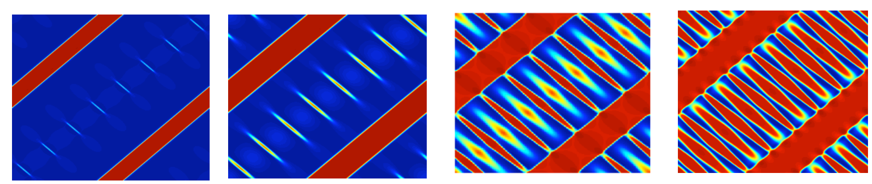
Solid-Solid Transformation | **SQUARE (High T, Austenite)** | **TO** | **RECTANGLE (Low T, Martensite)**

Thermal Nucleation of Martensite

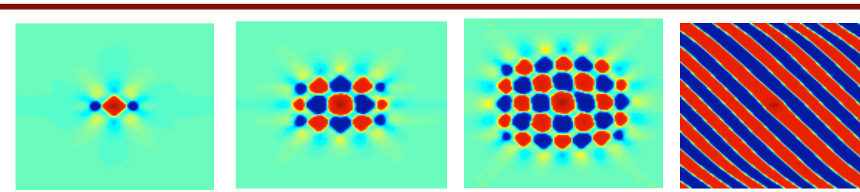
128x128



Local Sensitivity to Global perturbations (Uniform pressure)



Global Sensitivity to Local Perturbations (Local Stress) “Elastic screening”



cf. Diffuse X-ray “Butterfly”

(Vasilu-Doloc et al., *PRL* ‘00
Sinha et al., *PRL* ‘04)

Modeling Coupled Elastic, Spin, Charge Textures

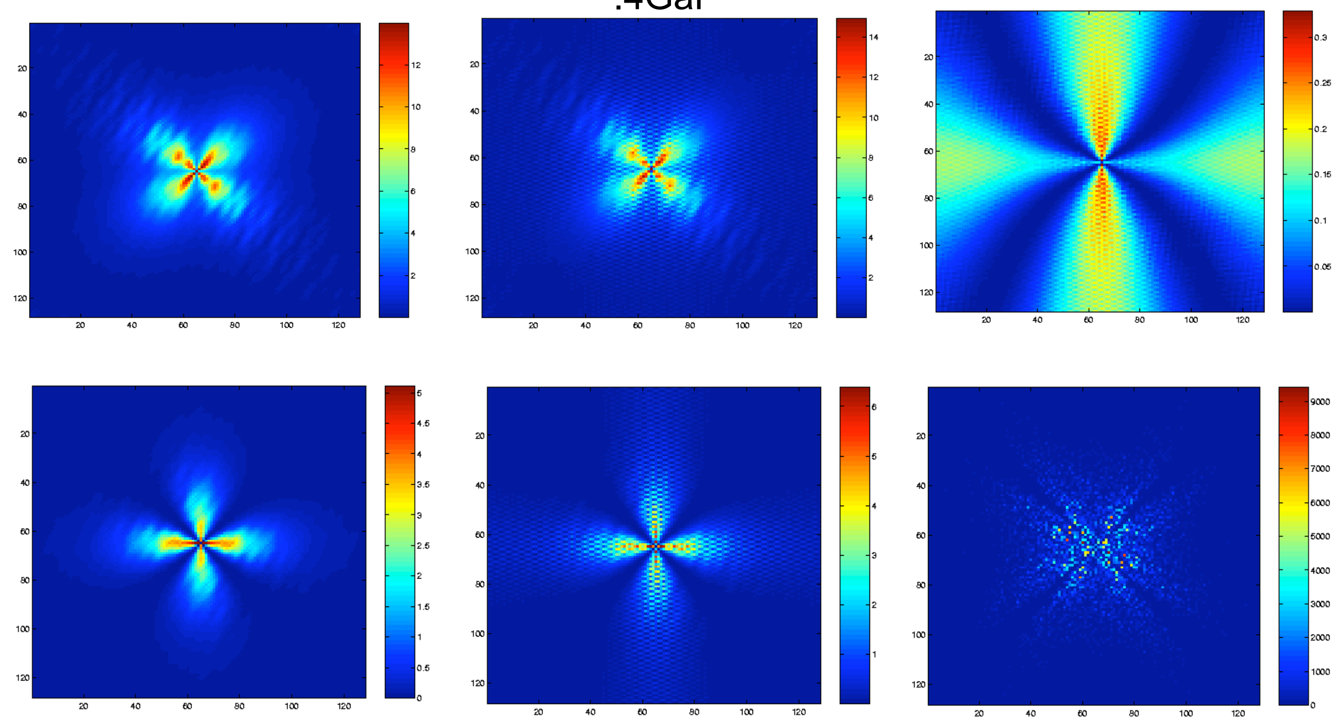
Magnetoelastic Polarons (cuprate parameters)

Pressure ~.4GaP

Difference

Deviatoric strain

Compressional strain



0 120

Europhys. Lett. **63**, 289 (‘03)

Modeling Coupled Elastic, Spin, Charge Textures

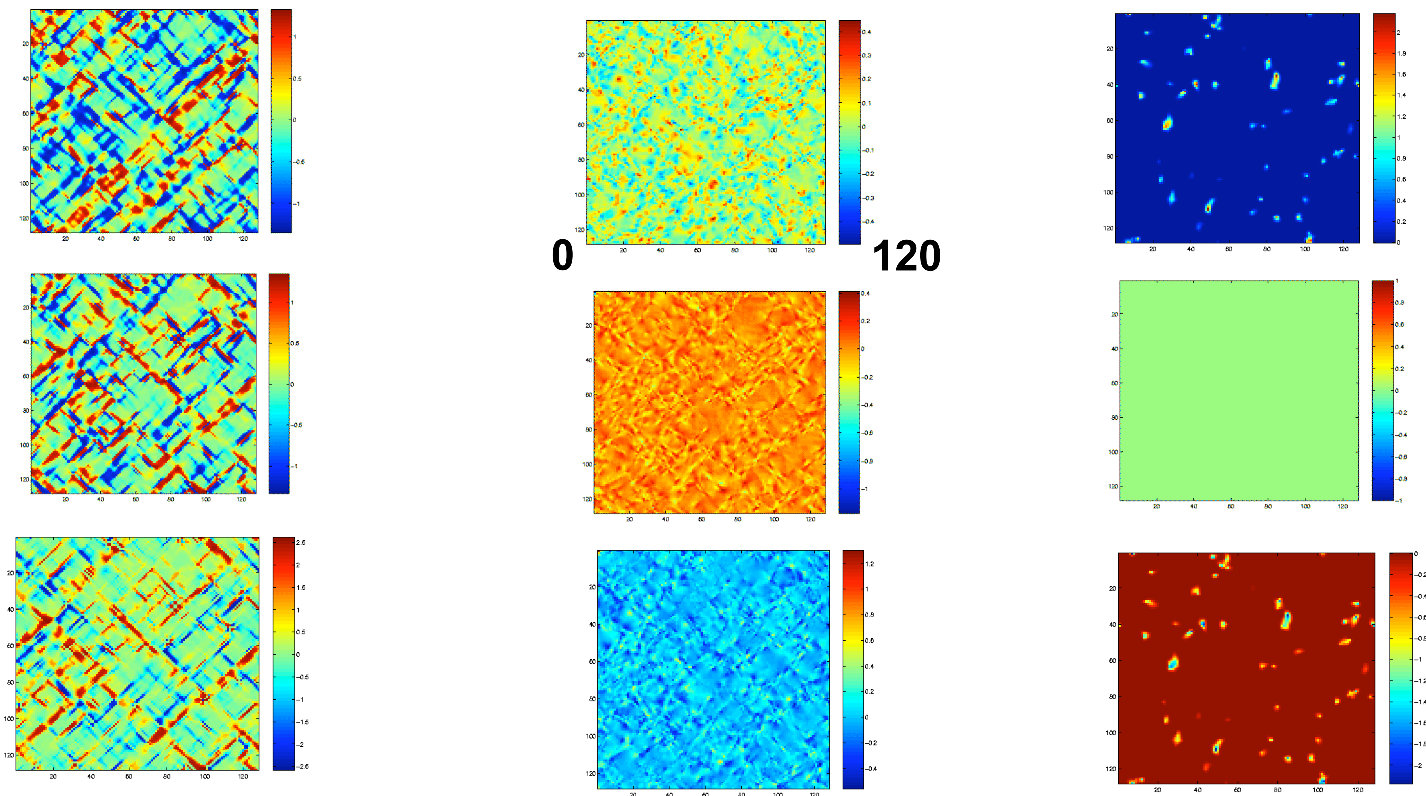
e.g., effects of pressure using cuprate parameters

Deviatoric strain | **Compressional strain** | **Magnetization**

Doping = 0.1
T = 0.5

With Pressure

Difference



Cross-responses; "correlated percolation" (x, T, M…)

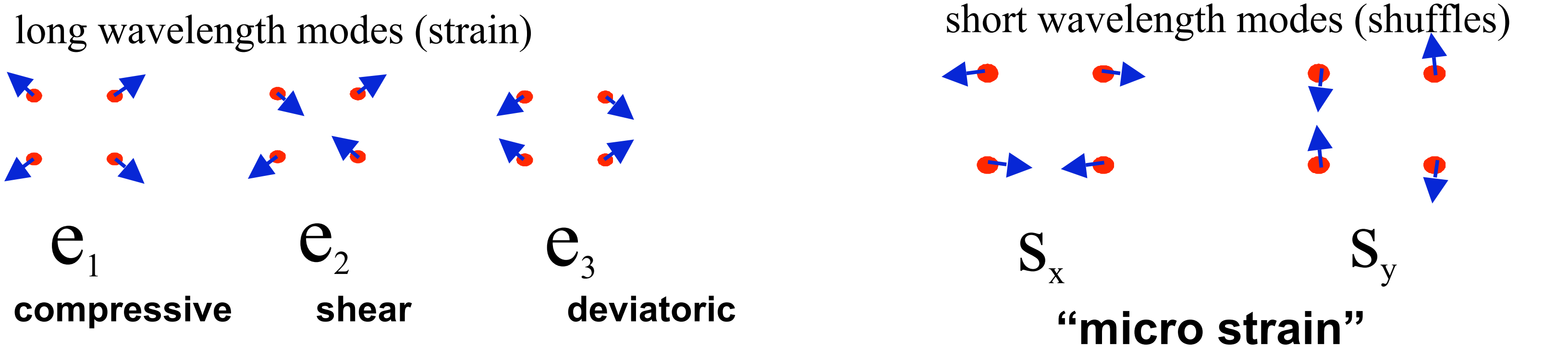
Europhys. Lett. **63,** 289 ('03)

Mode-based description of multiscale lattice distortion

- Recently developed and tested for twin/antiphase boundary
  (Ahn, Lookman, Saxena & Bishop, *PRB*, 2003/2005)

- Use atomic-scale modes instead of displacements,

Example: complete modes for 2D square lattice



- Constraints → long-range anisotropic interaction automatically included

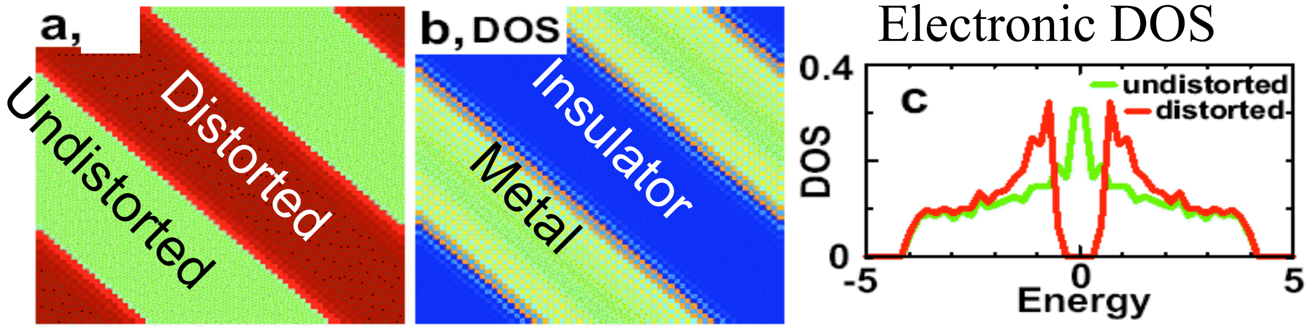
- Convenient for **multiscale** description (atomic **nano** ~ **micron** continuum)

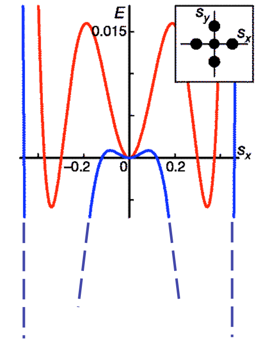
Application to CMR model :
Ahn et al., *Nature* **428**,401 (2004)

Results for deep local minimum case

Stable distortion pattern (S_x^2-S_y^2)

Electronic DOS

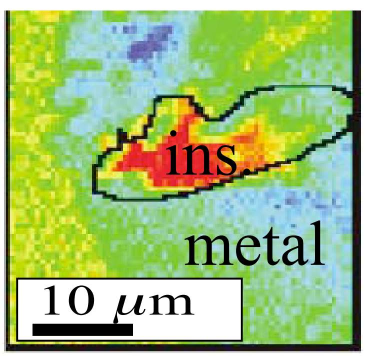




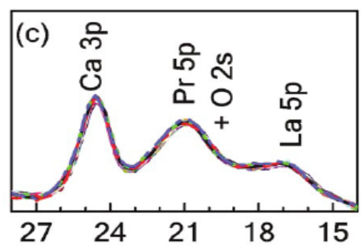
Ahn et al., *Nature* **428**, 401 ('04)

Photoelectron spectroscopy

(Sarma et al., *PRL* '04)



10-micron scale M/I domains



Binding energy (eV)

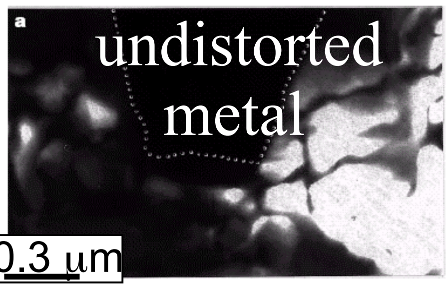
Intensity @ many regions

No chemical heterogeneity over 0.5 micron

Chemical heterogeneity?
Not required for stable M/I domains

Micrometer-scale heterogeneities in manganites

Dark field image

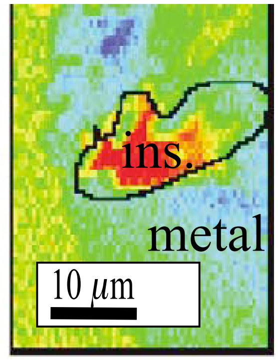


distorted
insulator

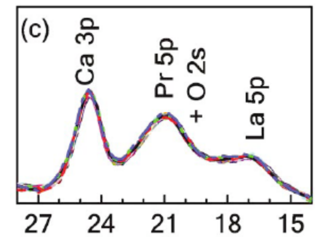
$La_{1/4}Pr_{3/8}Ca_{3/8}MnO_3$

T < 120 K
(Uehara et al., *Nature* '99)

Photoelectron spectroscopy



Intensity @ E_F



Binding energy (eV)
(Sarma et al., *PRL* '04)

Intensity
@
many
regions

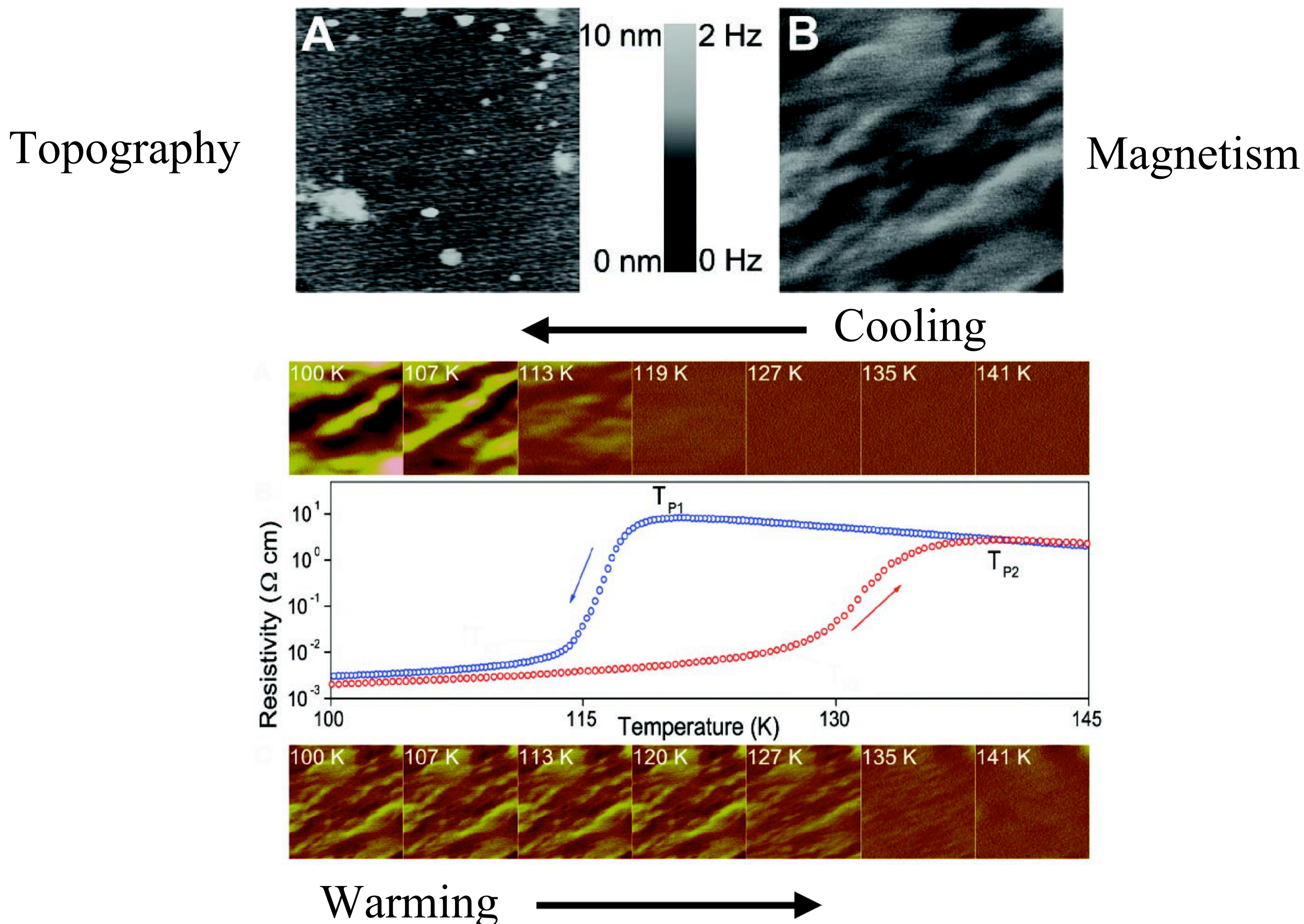
No chemical inhomogeneity
over submicron scale
→ Intrinsic effects

submicrometer scale

10-micrometer scale

- Metallic and insulating phases co-exist with sharp interfaces
- Precursor short-range order and quasi-elastic scattering
- Hysteretic, glassy dynamics and metastability
- T, M, Photo-induced metal-insulator transitions

Topographic and Magnetic Images of $La_{0.33}Pr_{0.34}Ca_{0.33}MnO_3$ At T = 120 K of a 7.5 x 7.5 μm area



Zhang et al., *Science* **298**, 805 (2002)

Magnetic imaging of a supercooling glass transition in a weakly disordered ferromagnet

Weida Wu[1], Casey Israel[1], Namjung Hur[2*], Soonyong Park[2], Sang-Wook Cheong[2] and Alex de Lozanne[1]

[1]Department of Physics, University of Texas, Austin, Texas, 78712

[2]Department of Physics and Astronomy & Rutgers Center for Emergent Materials, Rutgers University, Piscataway, New Jersey, 08854

*Current address: Los Alamos National Laboratory, Los Alamos, New Mexico, 87545.

Spin glasses are founded in the frustration and randomness of microscopic magnetic interactions[1]. They are non-ergodic systems where replica symmetry is broken. While magnetic glassy behaviour has been observed in many colossal magnetoresistive manganites[2-6], there is no consensus that they are spin glasses[7]. Here, an intriguing glass transition in (La,Pr,Ca)MnO3 is imaged using a variable- temperature magnetic force microscope. In contrast to the speculated spin glass picture, our results show that the observed static magnetic configuration seen below the glass temperature arises from the cooperative freezing of the first order antiferromagnetic (charge ordered) to ferromagnetic transition. Our data also suggest that accommodation strain plays an important role in the kinetics of the phase transition. This cooperative freezing idea, successfully applied to structural glasses such as window glasses and supercooled liquids[8], may be applicable across many systems to any first-order phase transition occurring on a complex free energy landscape.

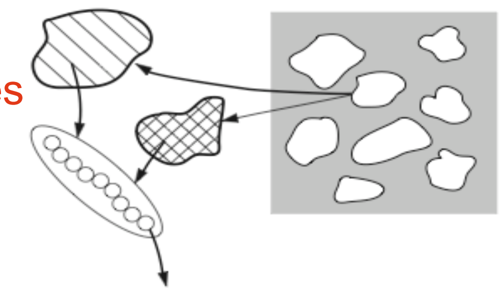
Transition Metal Oxides:

(and other "complex electron materials")

An Intrinsic Multiscale Framework

- Charge-spin-lattice (orbital) coupling essential
- Stable low-D electronically active regions (coherent patterns of "functional hotspots"; polarons, breathers, excitons) supported in a self-consistent elastic matrix:

Coupled Micro-Nano Scales



Self-organized "system" ; "engine"

cf. biological systems; covalent glasses

- Same local intra-unit-cell lattice distortions (buckling, ab-c coupling, …)

→ Local, anisotropic "chemistry"

Local Jahn-Teller polarons, lower bonding symmetry, dynamic charge transfer, magnetism, ferroelectricity, …

- And

→ Long-range, anisotropic elastic templates

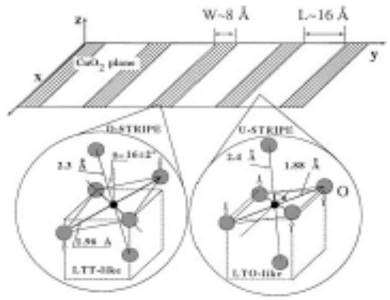
: pattern hierarchy [stripes, clumps, checkerboards, …]

: Low-D coherent electronic structures

Lengths (& time) scales coupled self-consistently

- Different probes detect different parts of the correlated heterogeneity (and different timescales)

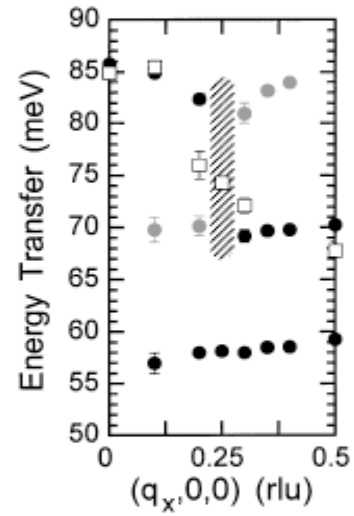
EXAFS



Bianconi
et al.

S(q, ω)

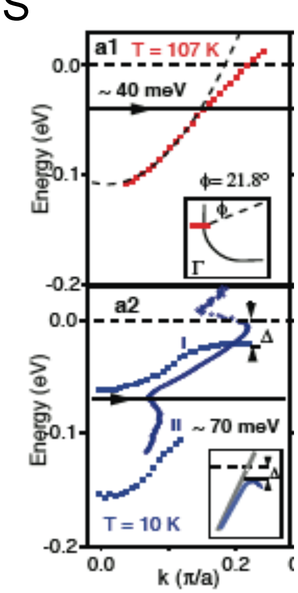
Egami
et al.

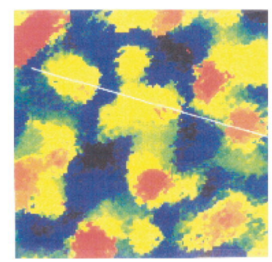


Many Experimental Indications of Spin, Charge, Lattice Heterogeneity: Nano, Micro, …

ARPES

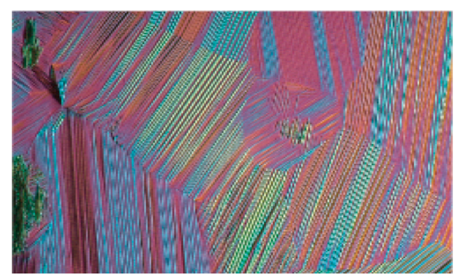
Shen
et al.





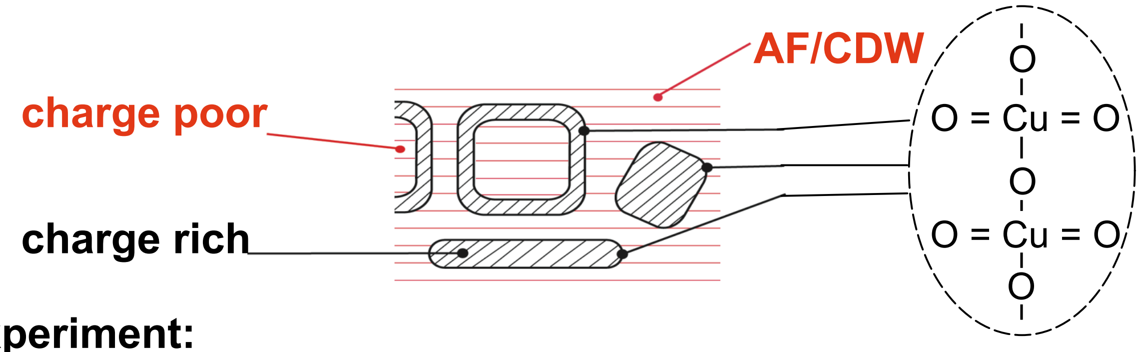
STS

Davis
et al.



HREM

Local Signatures of Charge Inhomogeneity in Doped Transition Metal Oxides: "Edge" (interface) Modes (Spin, Charge, Lattice)



$O_{\parallel} \sim$ 30-60 meV

$O_{\perp} \sim$ 70meV

Local "interface" modes
STRONG, LOCAL "el-ph"
[cf. S(q,ω) ARPES, σ(ω), NQR, ε(ω), EPR, STS, ...]

Experiment:

"Giant phonon anomalies" / mid-zone "splitting" in metal-oxygen bond stretching branches

e.g.,

Manganites:	Zhang et al., *PRL* (1999) Reichardt et al., *Physica B* **263,** 416 (1999)
YBCO:	McQueeney et al., *PRL* **82**, 628 (1999)
$Ba_{0.6}K_{0.4}BIO_3$:	Braden et al., *Physica C* **378,** 89 (2002)
$La_{1.69}Sr_{0.31}NiO_4$:	Tranquada et al, *PRL* **88**, 75505 (2002) etc.

Theory: Metal-oxygen charge-transfer essential

Yonemitsu et al., *PRL* **68** 965 (1992); *PRB* **47**, 12059 (1993)
Yu et al., *PRB* **57**, R3241 (1998)
McQueeney et al., *J. Phys. C* **12**, L317 (2000)
I. Martin et al., *PRB* **70,** 224514 ('04)

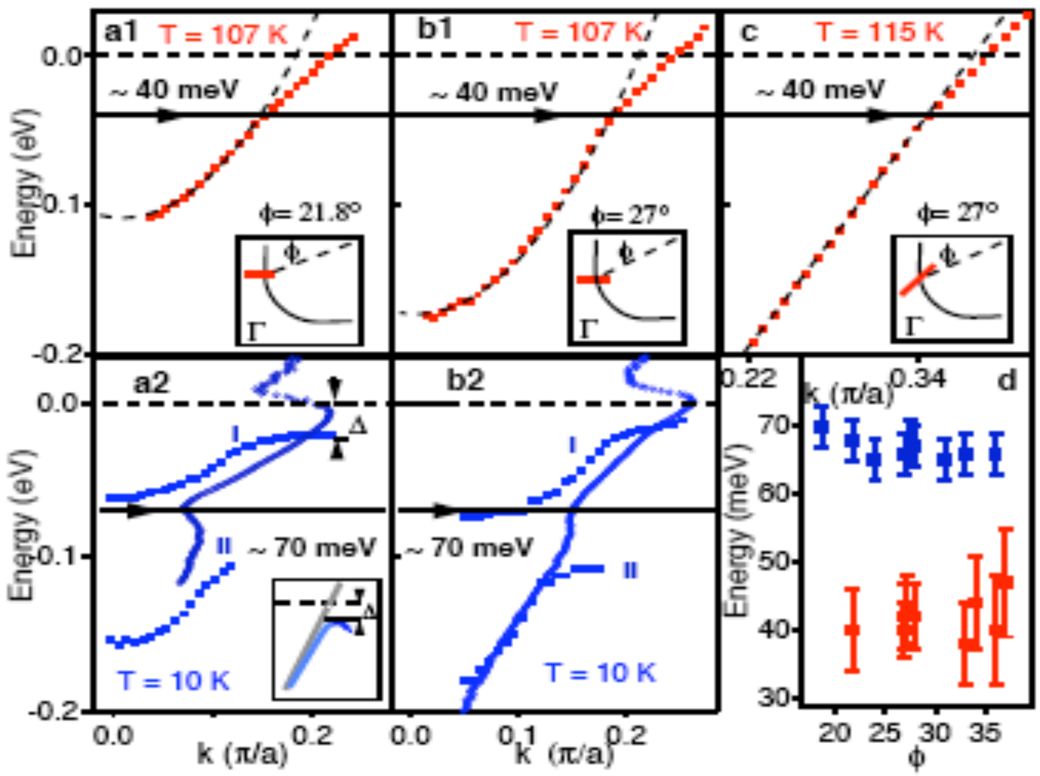
Note: Equivalent signatures for 1D CDW/AF - "Magnetoelastic Polarons" e.g., Gammel et al., *PRB* **45**, 6408 (1992); Huang et al., *PRB* **48**, R16148 (1993)

The ARPES Kink : Multiple "phonons"?

($Bi_2Sr_2Ca_{0.92}Y_{0.08}Cu_2O_{8+\delta}$; optimal doping)

Buckling
?
Longitudinal
Edge Mode

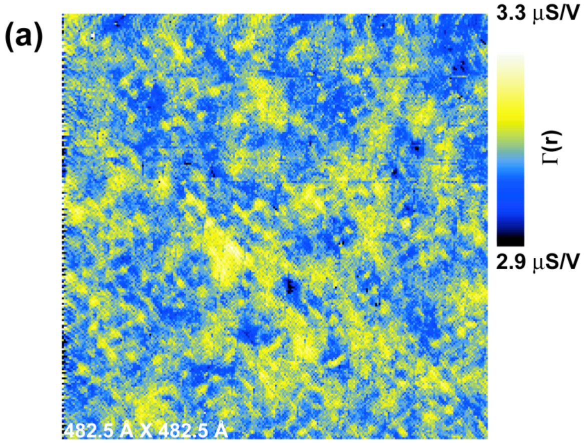
1/2 - Breathing
?
Transverse
Edge Mode

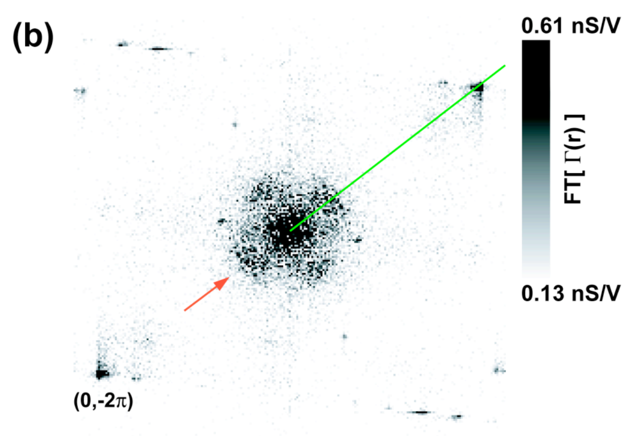


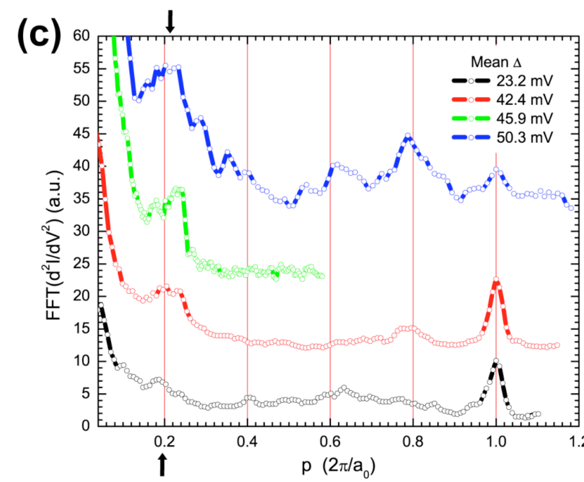
Cuk et al, cond-mat/0403521

Nanoscale Electron-Lattice Interactions in $BiSr_2CaCu_2O_{8+\delta}$

J. Lee et al., (Davis Group, Cornell; http://theory.lanl.gov)







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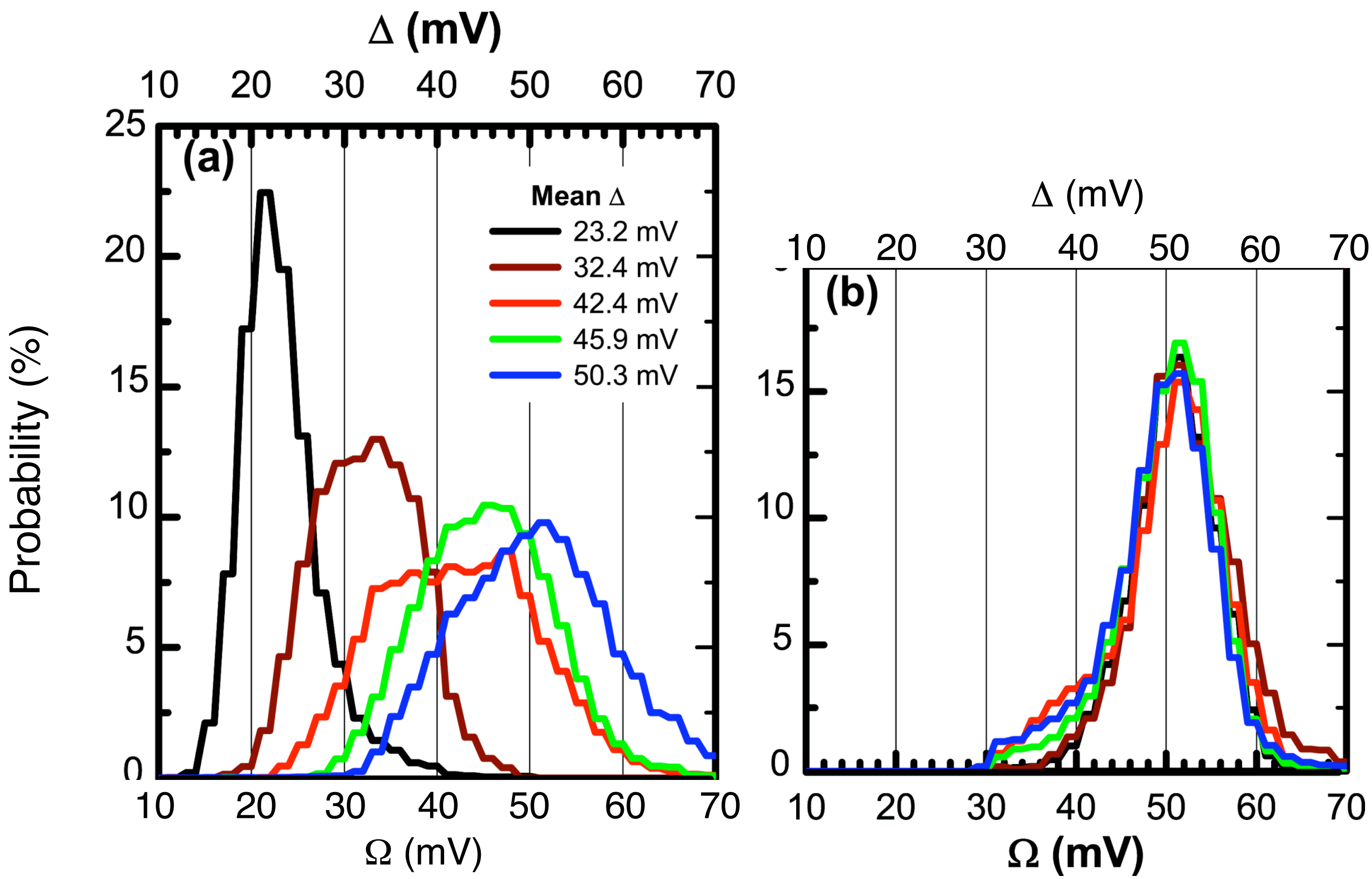
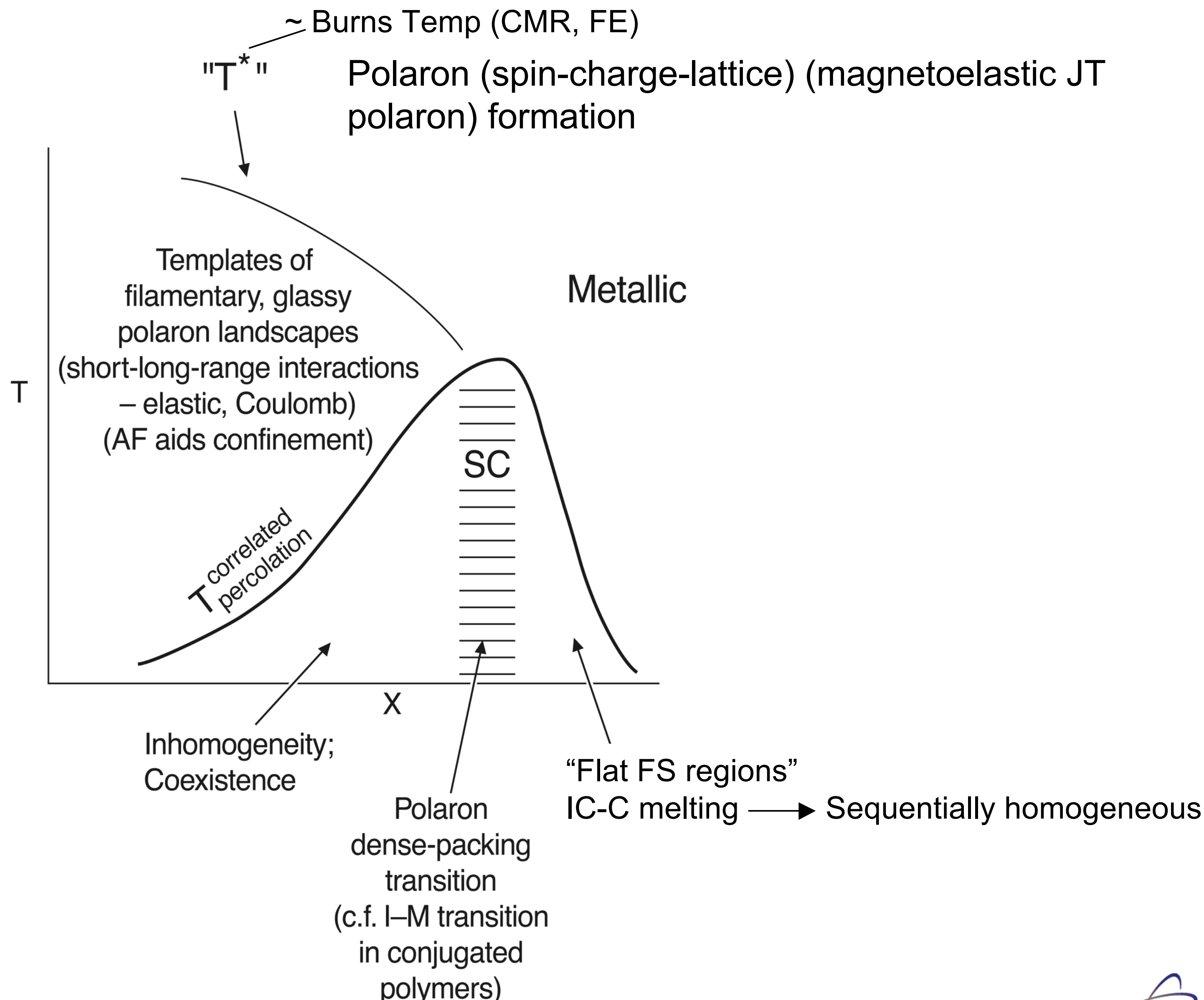


"Phase Diagrams" and HTCs



Elasticity (Constraint)-Controlled Electronics in Directionally-Bonded Materials

(inorganic, organic, bio)

Symmetry-restricted strain coupling to electronic wave functions **[P.E. $\gtrsim$ K.E.]**

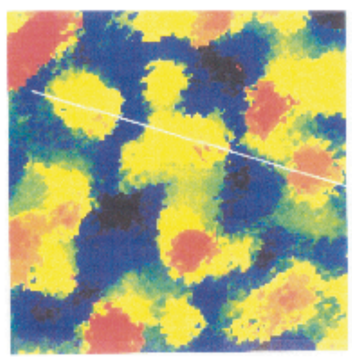
- Charge Transfer (ferroelectric dipole)
- SC, Magnetic (transition-metal oxides; VO_2; Laves; actinides, ...)
- Organics (conjugated polymers; mesoporous molecular structures, ...)
- Bio (DNA bubbles; rafts, ...)

- Global consequences of local constraints (frustration)

→ Inhomogeneous (local, mesoscopic) electronic & structure props
→ Elasticity-induced electronic symmetries

NANO

(STS)



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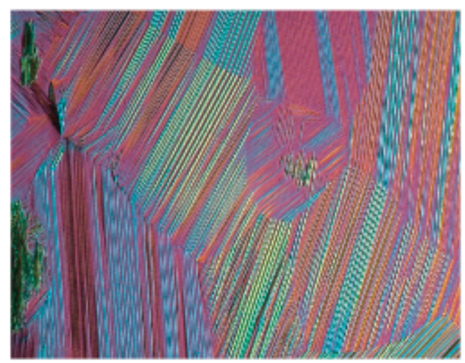


MICRON

(HREM)

e.g., *PRL* **91**, 057006 ('03); *Nature* **428**, 401 ('04); *PRB* ('06)

Atomic Scale Elastic Textures Coupled to Electrons in Superconductors

(J-X Zhu et al., *Phys. Rev. Lett.* **91**, 057004 (2003))

- Bogliubov-de Gennes on elastic template patterns

➡ SC propagated via elasticity
anisotropic, long-range

c.f. "Giant proximity" effects in HTC multilayers

e.g. I. Bozovic et al. (SNS)
Ch. Bernhard et al. (GMR)

➡ Texture-induced pairing symmetry
(s, d mixtures …)

A Common Sequential Scenario in "Complex" "Strongly Correlated" Materials

- Local constraints and long-range consequences where P.E. $\gtrsim$ K.E.
- Short-range-long-range competition
- Mesoscopic order (clumps, filaments, …)
- Landscapes, metastability, glassiness, …)
- Mesoscopic coexistence / phase separation, …
- Stable Low-D (Self-Assembled) Physics

Materials

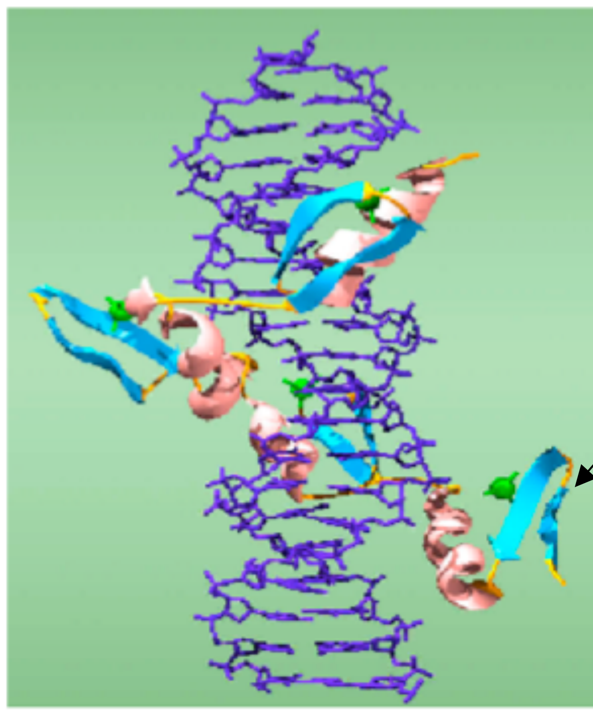
- Transition metal oxides (d - orbitals) [HTC (cuprates, bismuthates), CMR, ferroelectrics]
- Nickelates, hexaborides, cobaltates, spinels, Laves phase, zeolites, VO_2, V_2O_3, WO_x, …
- Heavy fermions (f - orbitals)
- CDW dicalcognenides
- Multi-ferroics (magnetism + ferroelectricity)
- High-spin-low-spin complexes
- Covalent glasses, S_iO_2, …
- Metal-insulator transitions in inversion layers
- Organics (conducting polymers, charge transfer salts, superconductors)
- Bio-macromolecules (DNA, proteins)

DNA as Soft Electronic Matter

- constraints and networks -

With K.Ø. Rasmussen, G. Kalosaka, N. Voulgarakis, S. Ares, Z. Rapti, A. Smerzi, A. Usheva, and C.H. Choi

See: *J. Chem. Phys*. **118**, 3731 (2003): *Nucl. Acid. Res*. **32**, 1589 (2004); *Nano Lett*. **4**, 629 (2004); *Europhys. Lett*. **68**, 127 (2004); *PRL* **94**, 35504 (2005); *Europhys. Lett. (2006)*



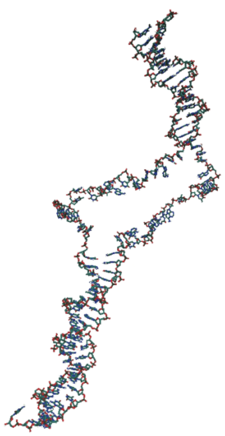
Polymerase (transcription)

DNA as Soft Electronic Matter

- constraints and networks -

- Specific **local**, **dynamic**, **nonharmonic** conformational deviations ('hotspots") from average structure, control distinct macroscopic functions in **hard, soft, biological** matter (e.g., protein diversity, rafts, …)

- DNA is intrinsically "soft" because of nonlinear base-pair stacking interactions: constraints



→ nontrivial entropic (T) effects

→ Long-range coherence / "interactions"

→ "elastic" precursors to first-order nucleative denaturation transition

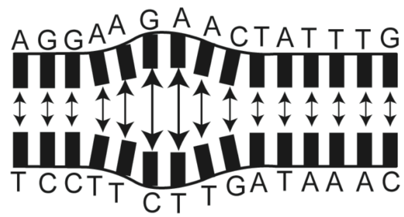
→ Large amplitude, local, coherent base pair openings: "bubbles": rare-event statistics
(only in the "living" T-range!)

- Base-pair sequence constitutes "colored disorder" which selects bubbles and their locations

- Relevance for transcription initiation, repair, mechanical unzipping …?
[Choi et al, *Nucleic Acids Research* **32**, 1584 (2004); B. Alexandrov et al., DNA Repair **5**, 863 (2006)]

Peyrard-Bishop-Dauxois Model

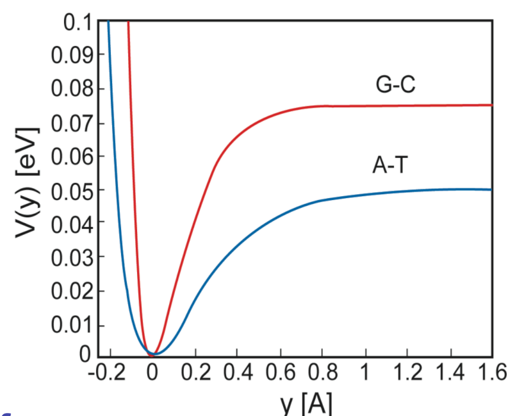
M. Peyrard and A.R. Bishop, *PRL* **62** 2755 (1999); T. Dauxois, M. Peyrard, and A.R. Bishop, *PRE* **47** R44 (1993).



Coherent openings
"bubbles"

$$H = \sum_n \frac{1}{2} m \left(\frac{dy_n}{dt} \right) + V(y_n) + W(y_n, y_{n-1})$$

Base pair potential: $V(y_n) = D_n\,(\exp[-a_n y_n] - 1)^2$



Stacking constraints/entropic effects:

$$W(y_n, y_{n-1}) = \frac{k}{2}\left(1 + \rho \exp[-\beta(y_n + y_{n-1})]\right) \times (y_n - y_{n-1})^2$$

$D_n = 0.05eV$, $a_n = 4.2A^{-1}$ *for AT base pair*

$D_n = 0.075eV$, $a_n = 6.9A^{-1}$ *for GC base pair*

Wild & Mutated

e.g. Adeno Associate Viral Promoter (AVV P5)

Wild type

-46 (start) · **-21** (above GAGTGAGCGA)

GTGGC CATTTAGGG TATATATGGCC GAGTGAGCGA GCAGGATCTC CATTTTGACC GCGAAATTTG AACG

+1 (below CATTTTGACC) · **+23** (end)

Mutant — **GC**

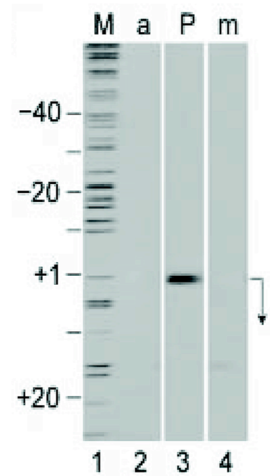
-46 (start) · **-21** (above GAGTGAGCGA)

GTGGC CATTTAGGG TATATATGGCC GAGTGAGCGA GCAGGATCTC CATTTTGACC GCGAAATTTG AACG

+1 (below CATTTTGACC) · **+23** (end)

Mutation removes transcription and large bubbles at initiation site

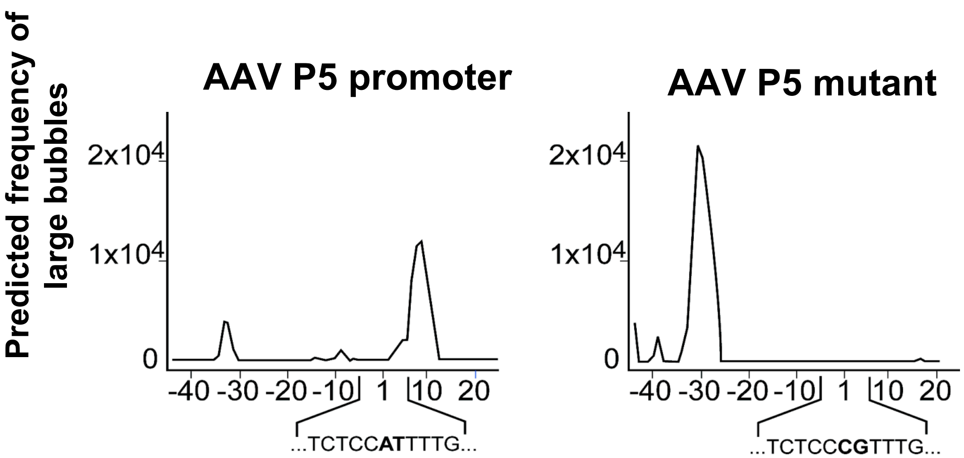
Choi et.al., *Nucleic Accids Res.* **32,** 1584 (2004)



M: sequence marker

P: RNA transcription product

(Room Temperature)

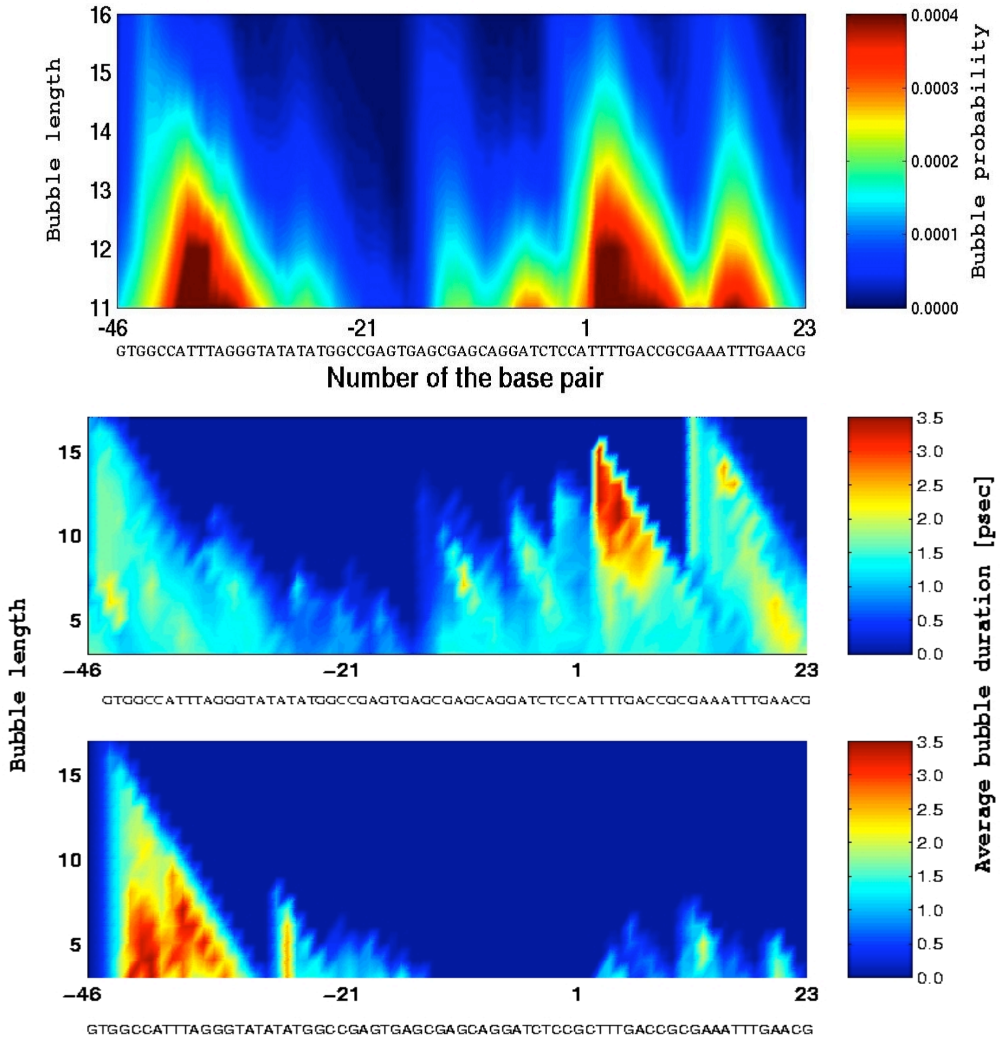


Bubble Statistic and Dynamics in Double-Stranded DNA

B. S. Alexandrov, L.T. Wille, K.Ø. Rasmussen, A.R. Bishop, and K.B. Blagoev

arXiv:cond-mat/0601555

e.g. Adeno Associate Viral (AAV) P5 promoter



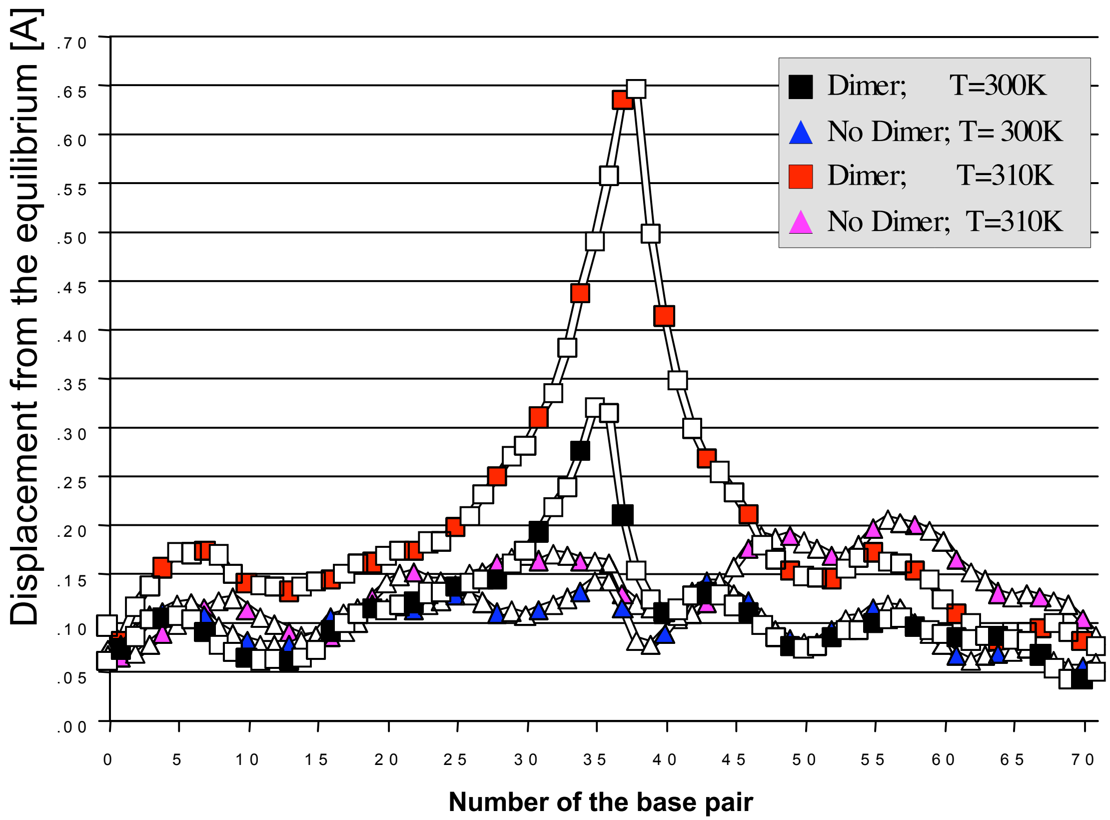
$$P_n(l,tr) = \left\langle \frac{1}{t_s} \sum_{q_n^k=1}^{q_n^{k\,max}(l,tr)} \Delta t[q_n^k(l,tr)] \right\rangle_M$$

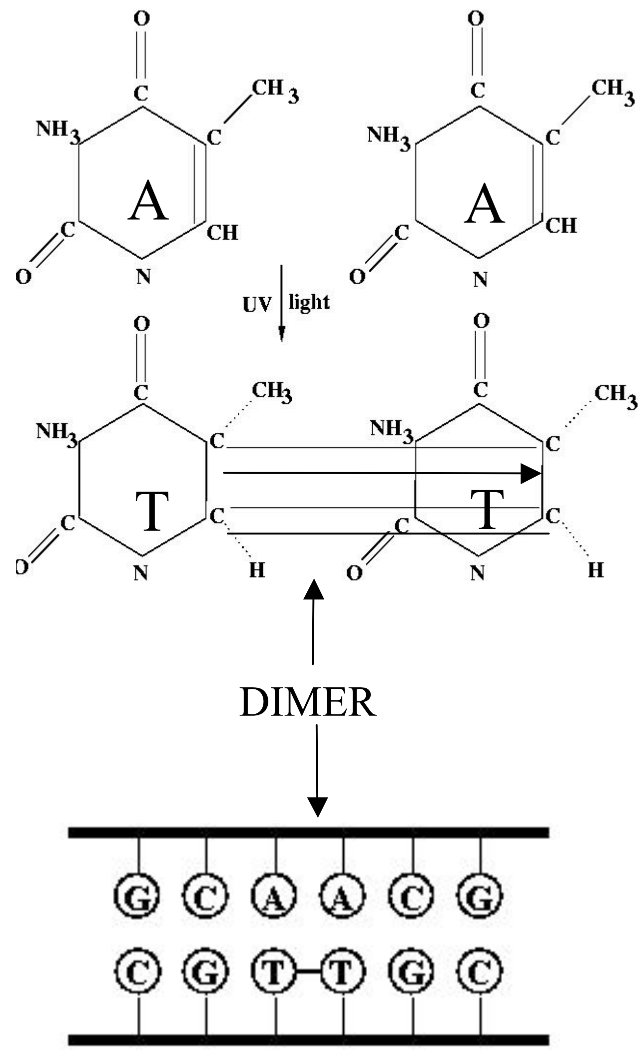
- ***l*:** bubble length
- ***tr*:** bubble amplitude
- $q^k{}_n(l, tr)$**:** # bubbles with amplitude ***tr*,** spanning ***l*** consecutive base-pairs beginning at the ***n***th base-pair in the ***k***th simulation.
- $\Delta t[q^k{}_n(l, tr)]$: existence time of $q^k{}_n(l, tr)$ 'th bubble.
- t_s [1 - 2 nsec]: duration of single simulation
- ***M*:** # of the simulations

$$\mathrm{ABD}\,(n,l,tr) = \left\langle \frac{\sum_{q_n^k=1}^{q_n^{k\,max}(l,tr)} \Delta t[q_n^k(l,tr)]}{\sum_{q_n^k=1}^{q_n^{k\,max}(l,tr)} q_n^k(l,tr)} \right\rangle_M$$

Self-healing mechanism in DNA: UV-induced dimer defects

K.B. Blagoev, B.S. Alexandrov, E.H. Goodwin, and A.R. Bishop, DNA Repair (2006) ***5****, 863 ('06)*

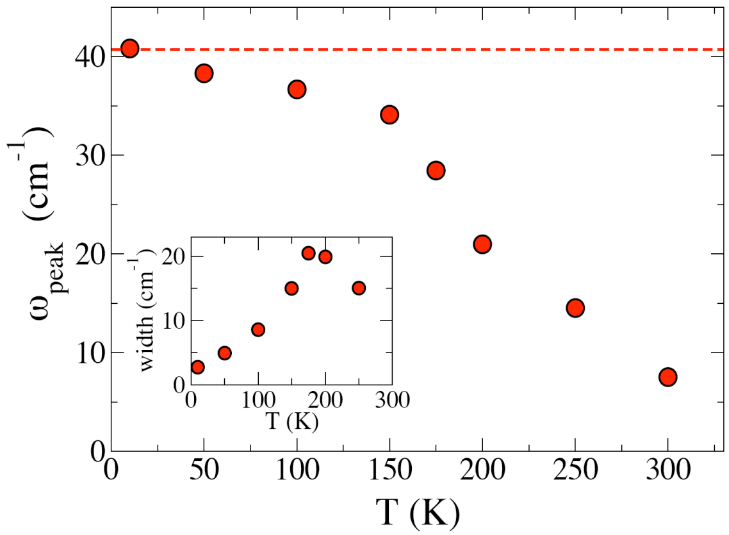


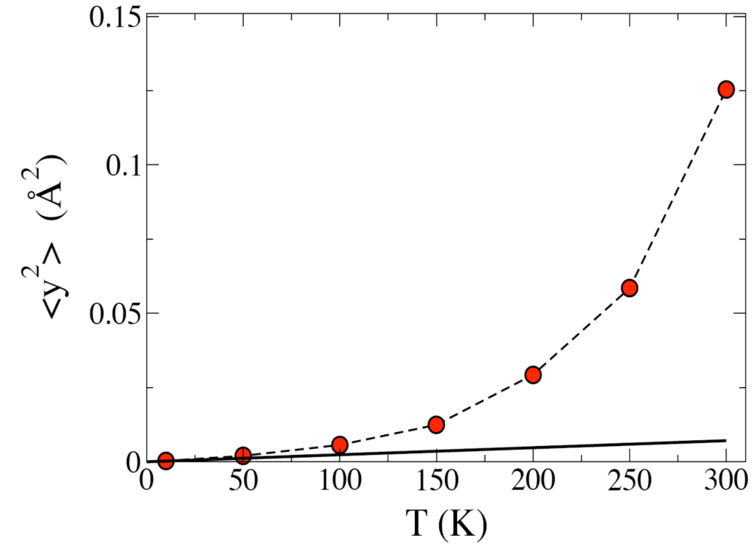


Average verticle size of bubble with min length 3 bp for a random sequence with and without dimer

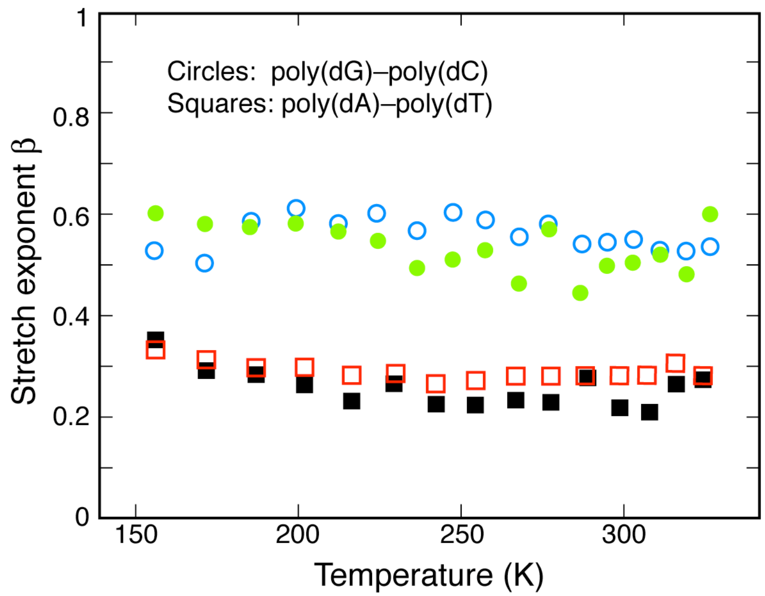
GCAGATCAAGGTGCGAGTAGTGTGTTACACTAGCGTTGCGGTTACAATGGCATGATACATCGACGAAAGTCCG

"Glass Transition" in DNA?





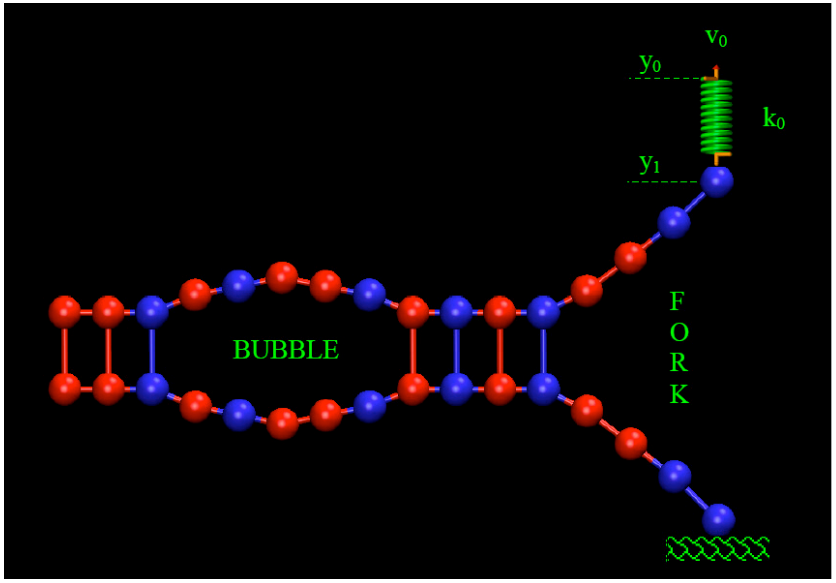
Nano Lett. **4**, 629 (2004)

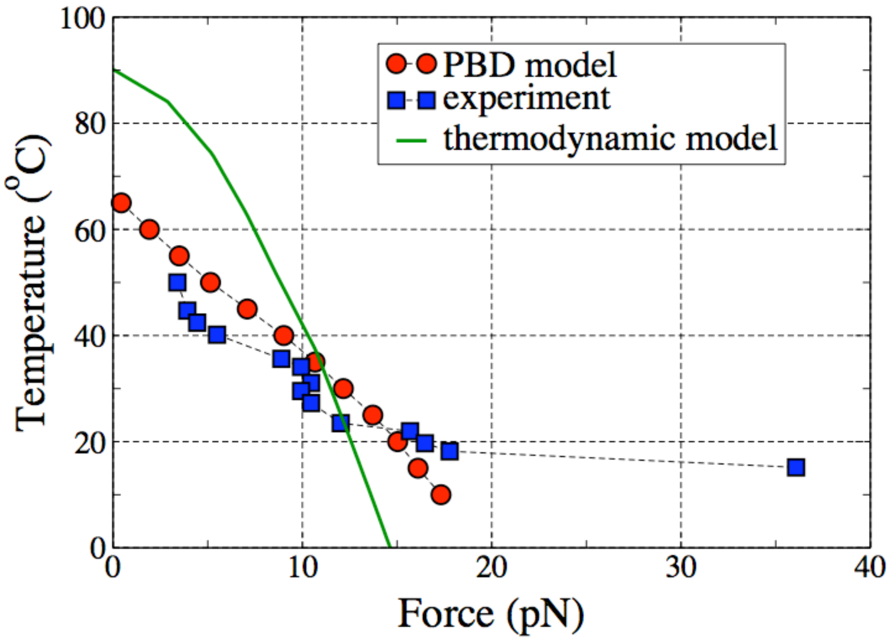


T-dependence of "Debye-Waller" factor, structure factor and stretched exponential exponents.

G. Kalosakas et al., (2006)

Unzipping DNA





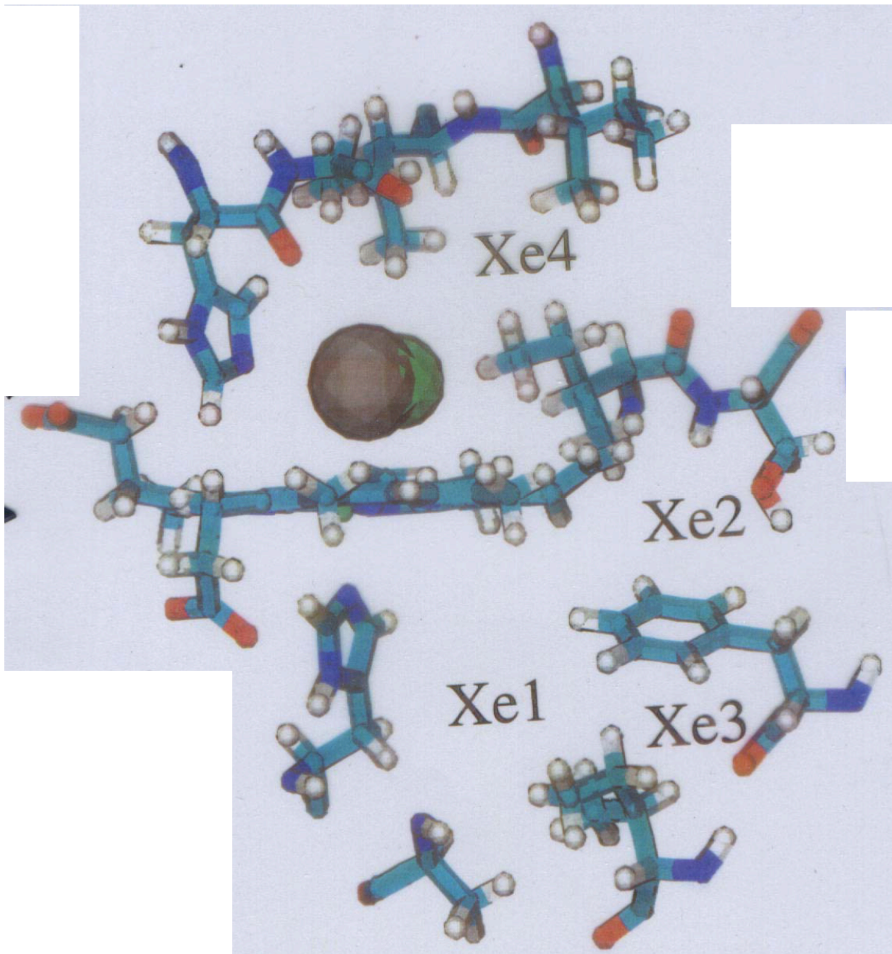
Experiment: Danilowicz et al, PRL **93**, 078101 (2004)

PBD model: Voulgarakis et al, to appear in PRL (2006)

Biology: Research Frontiers Post Gene Sequencing?

e.g. Biology “systems”: Multiple connected functions

e.g. Beyond <Structure>:
Functional Substates (Dynamic, Transient “Landscapes”)



Myoglobin

Low/High Spin

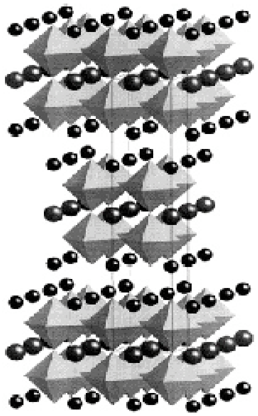
↕

Heme Doming

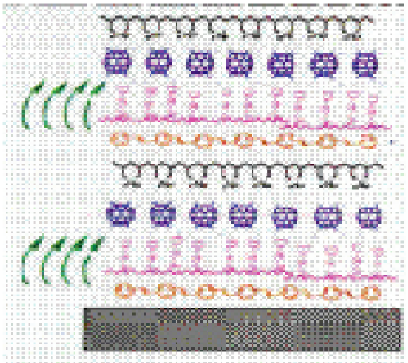
X-Ray Crystallog.
(Berendzen *et al.* 1998)

"Strongly Correlated" Electronic Matter:
Multiscale Tunability of Electro-Elastic Matter

- New concepts: new technology



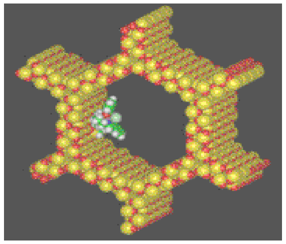
Layered perovskite oxides



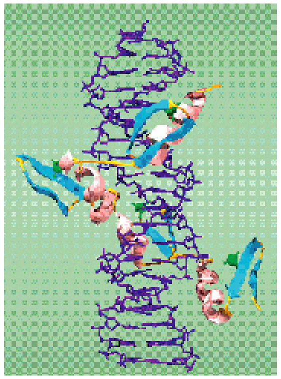
Organic self-assembly

- Deformable Building Blocks (complex unit cells/molecules) and Constraints
  - Functioning at the nonhomogeneous (hard-soft) edge!
  - Multiscale Networks: Correlated "hot spots", intrinsic nanoscale structure and electronics

Adaptive intermediate phases (e.g. *PRL* **94**, 208701 ('05))



mesoporous organic inorganic hybrids



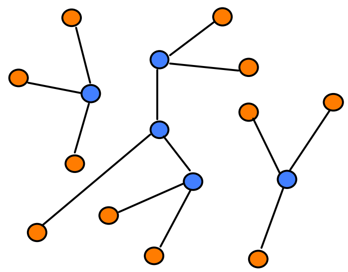
Adaptable Network

(Barré et al., *Phys. Rev. Lett.* **94,** 208701 ('05))

Stress costs energy: allow network to adapt to avoid stress

Degree of randomness

$$a = \frac{N_{11}}{N_{11}^{*}}$$ ← Random cluster value



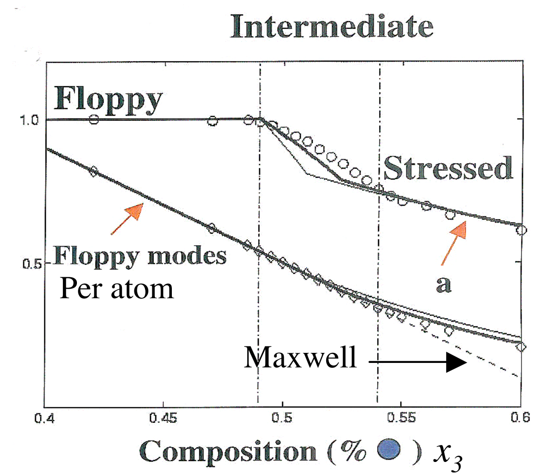
N_{11}

N_{13}

N_{33}

$F = H - TS$

Redundant constraints ← → $\Omega\ (a, x_3)$



Include correlations

- Intermediate adaptive phase from proximity of 1st order transition and entropy (covalent glasses, oxides, protein folding?, computability? ….)

Materials Functioning Beyond the Bloch Theorem

- The “Non” science of local/mesoscopic structure and dynamics:
  - Beyond average, periodic, harmonic
- Origins, Measures, Consequences
- Nonthermal, nonlinear, nonadiabatic, noncontinuum, nonequilibrium, nonergodic
- Organic, inorganic, biological matter

The "Century of Complexity"

– Embracing, Understanding, Using –

e.g., Materials Science (Same path in Biology, etc.)

- Science of "**synthesis-structure-property**"
- **Complex materials structure** — intrinsic / engineered
- Coupled spin-charge-lattice (orbital); Local constraints; (dimensionality, interfaces, disorder)

➡ **Competing / coexisting length and/or time scales** (nonlinear, nonadiabatic, nonequilibrium)

➡ Multiscale Materials (Micro-Meso-Macro)

hiearchically connected functional scales

- "systems"
- "engines"
- "networks"

"soft" phases, local/meso states

function means dynamics

- coupled space/time
- spatio-temporal patterns
- glassy, metatstable, nonequilibrium, …

➡ **"Electro – Elastic" Matter ("multiferroic") (magnetic, photo, …)**