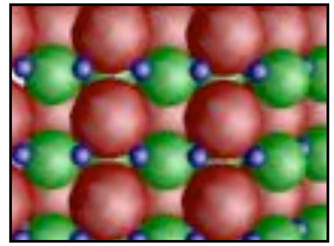
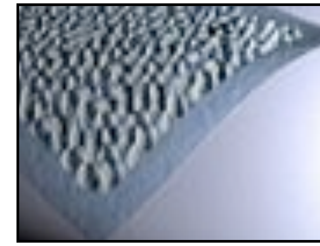
Materials design:

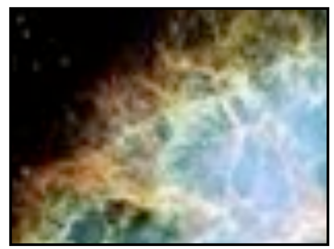
- continuous
- discrete
- information
- geometry
- regime



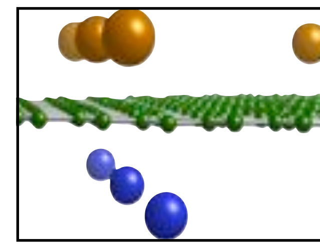
colloid GA



experimental computation

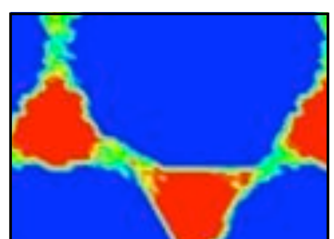


neutron star crust



topological frustration

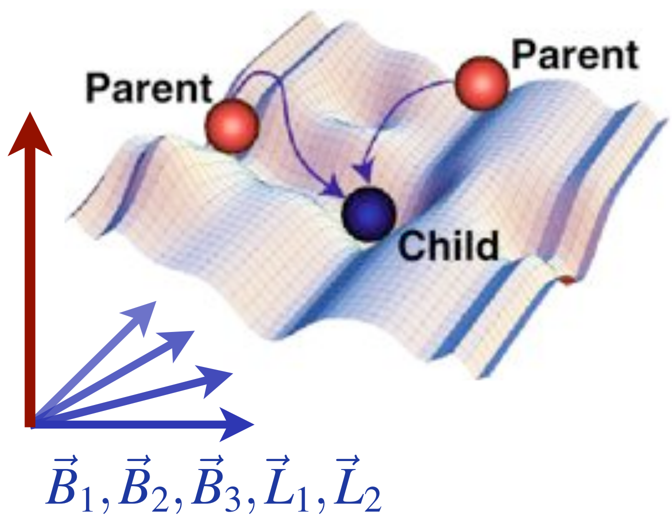
materials information

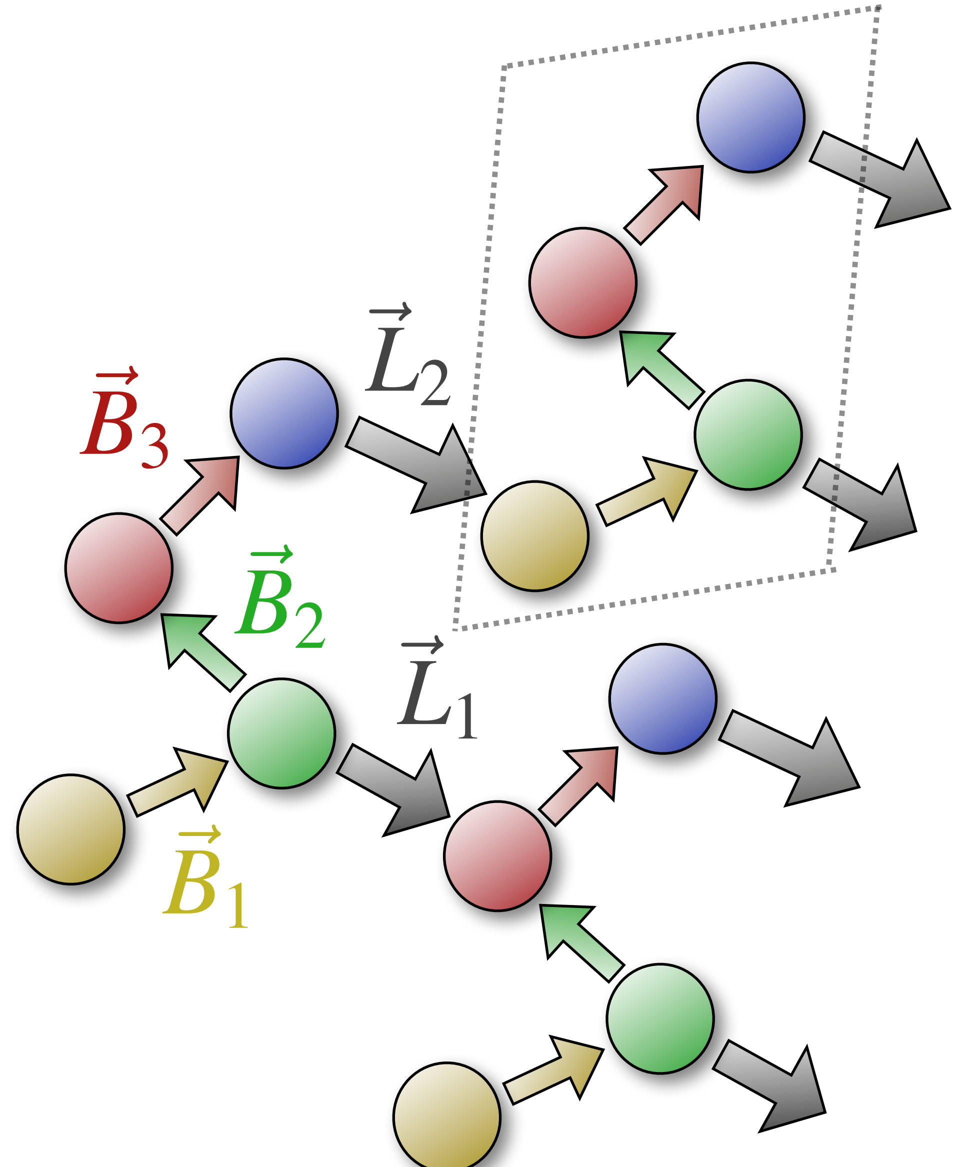


photonic crystal

cellulose twist

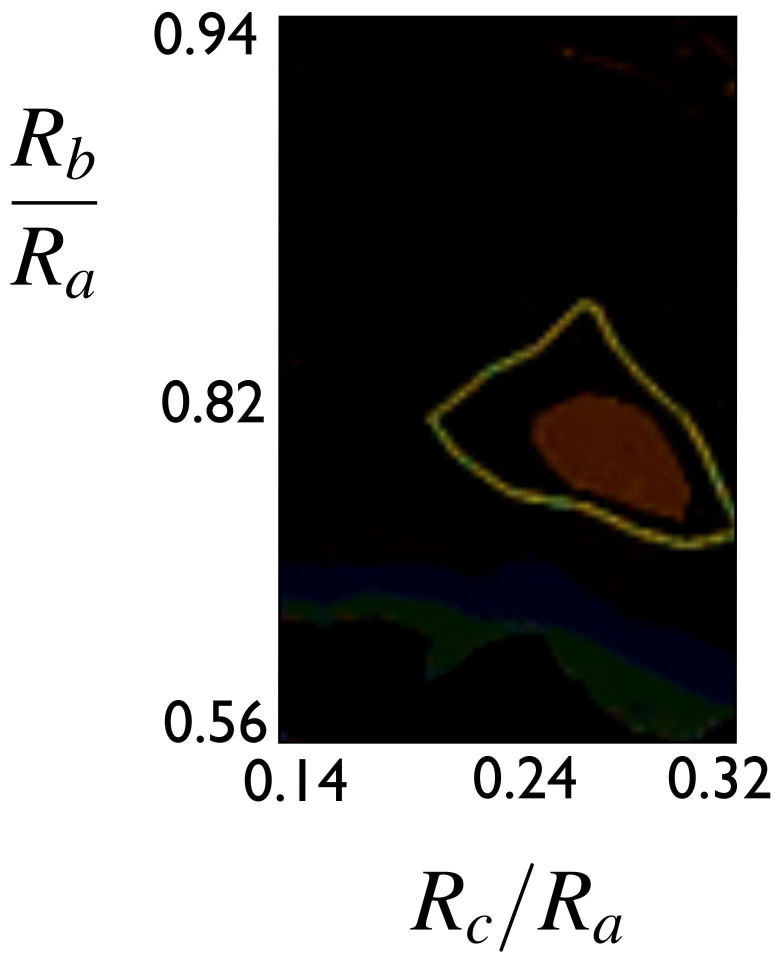
Optimization of colloidal crystalline packings

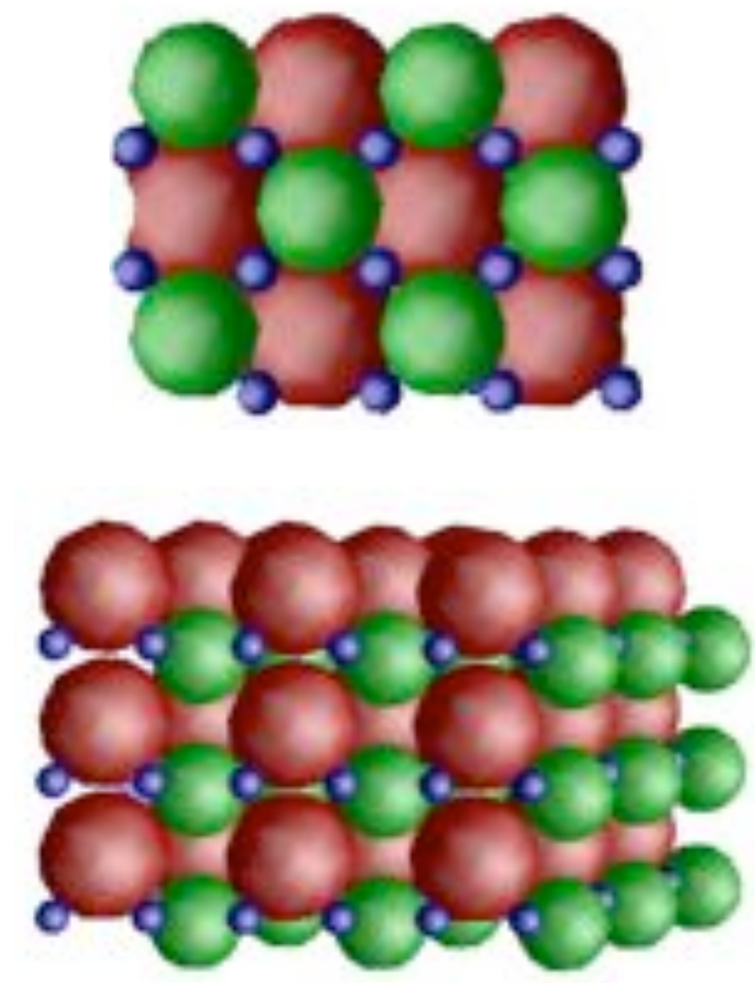




D. Stucke and V. H. Crespi, *Predictions of New Crystalline States for Assemblies of Nanoparticles: Perovskite Analogues and 3-D Arrays of Self-Assembled Nanowires*, Nanoletters **3**, 1183 (2003)

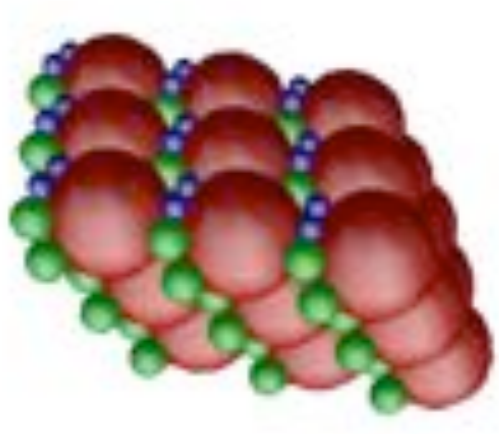
ABC_2

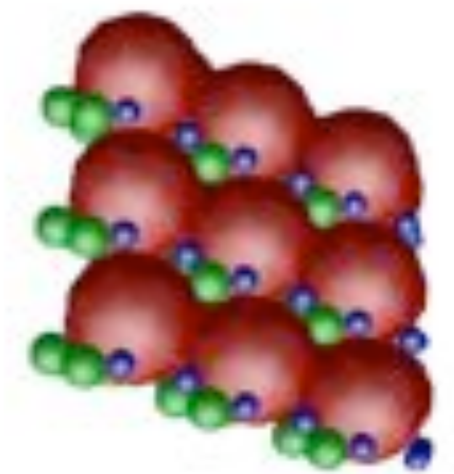


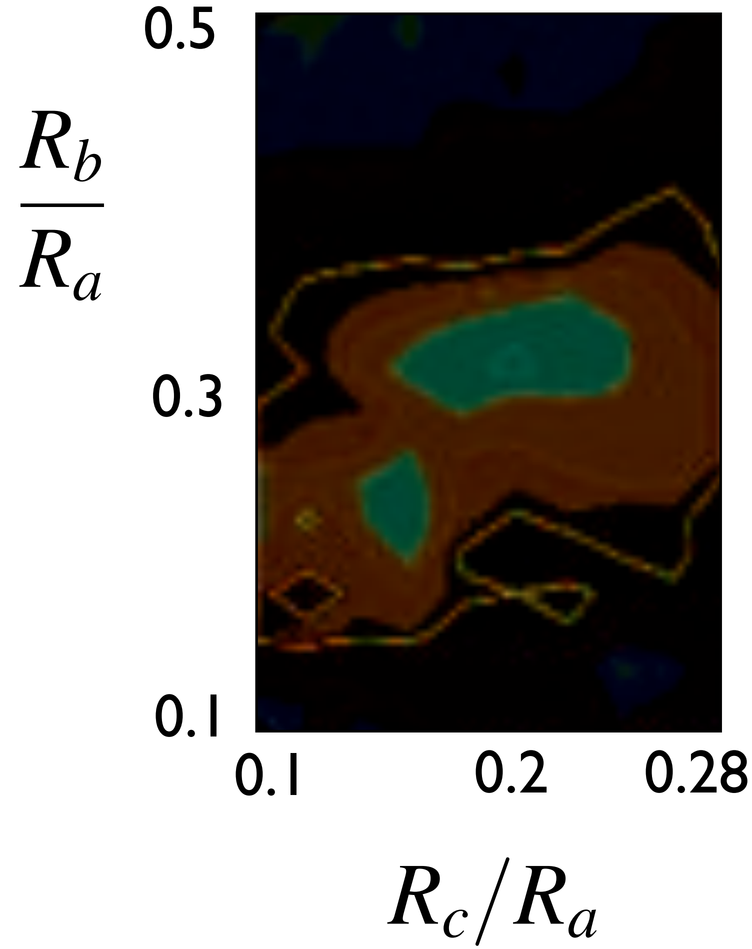


Perovskite without the apical oxygen

AB_2C_2

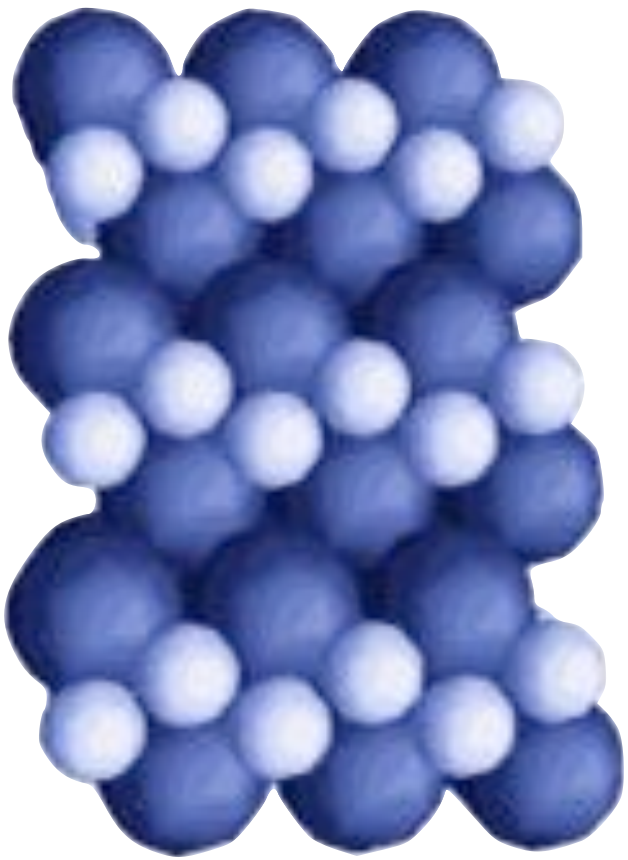






A packing fraction similar to perovskite,
but over a wider range of parameters

$(AB)_2$

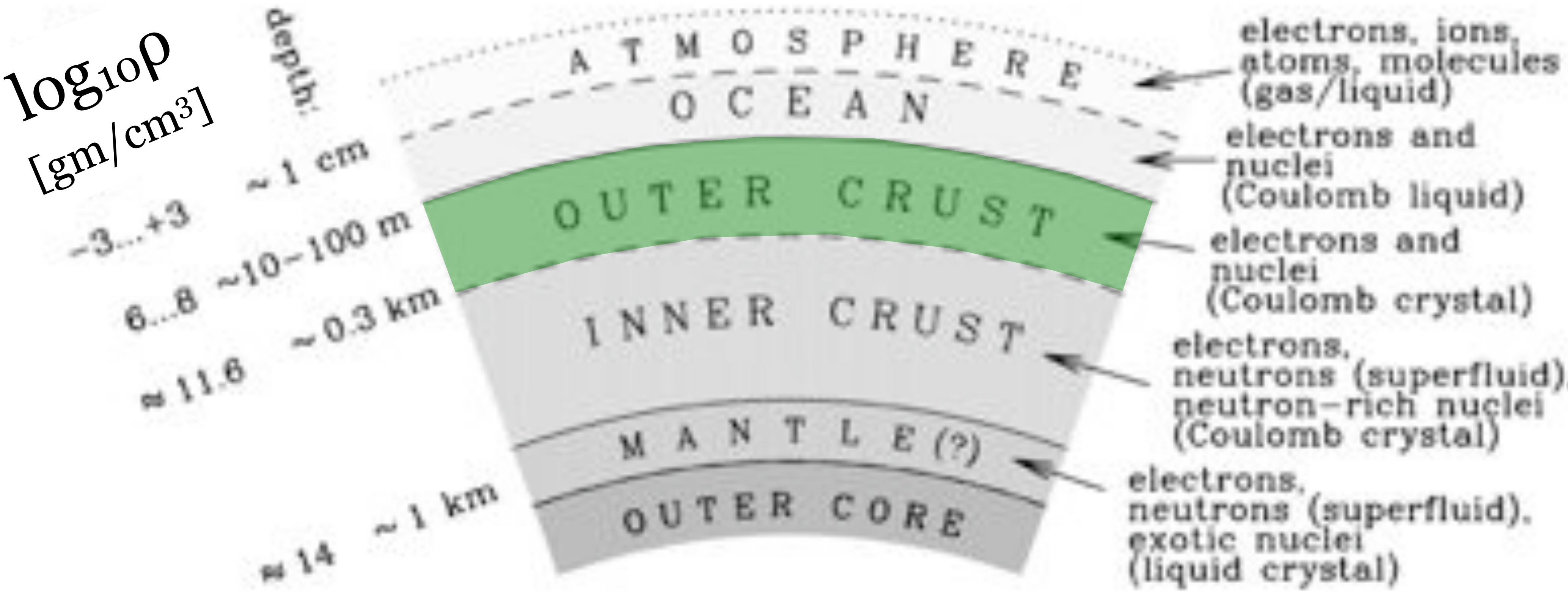


$$\frac{R_A}{R_B} \approx 0.6$$

A & B are bound into a dimer to frustrate phase separation

A three-dimensional array of "A" nanowires: Give nature a difficult problem and it finds a creative solution.


Really
condensed
matter
NASA



P. Haensel et al. 2007

Between pressure ionization and neutron drip:

$$\phi = \sum_{i<j} Z_i Z_j e^2 \frac{e^{-r_{ij}/\lambda}}{r_{ij}}$$

$\lambda \approx 1$ lattice spacing

10^4 g/cm^3 < P < 10^{11} g/cm^3

$\varepsilon_F > 0.5$ MeV

$T/\varepsilon_F = 10^{-3}$ to 10^{-1}

Jellium as a condensed matter physicist can only dream...

Crustal structure & composition:

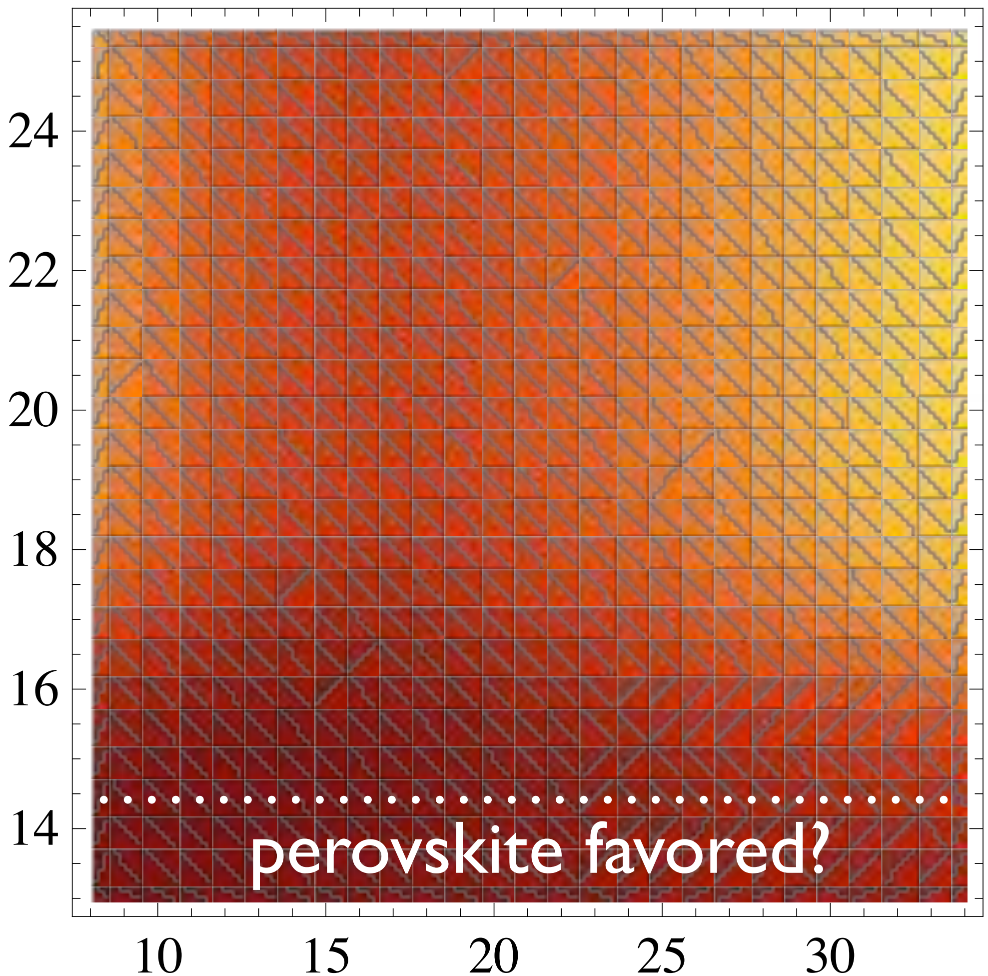
Molecular dynamics:
BCC or FCC

Fraction	Z
0.43	34
0.14	33
0.09	30
0.07	28
0.10	26
0.06	24
0.06	22
remainder	8 to 47

Simulated accretion nucleosynthesis

◂ C. J. Horowitz and D. K. Berry, Phys. Rev. C **79**, 065803 (2009)
▸ S. Gupta, E. F. Brown, H. Schatz, P. Möller and K-L. Kratz, Astrophys. J. **662**, 1188 (2007)

$\mu_{perovskite}/\mu_{fcc}$



$\log_{10} P$ [bar]

Z_B

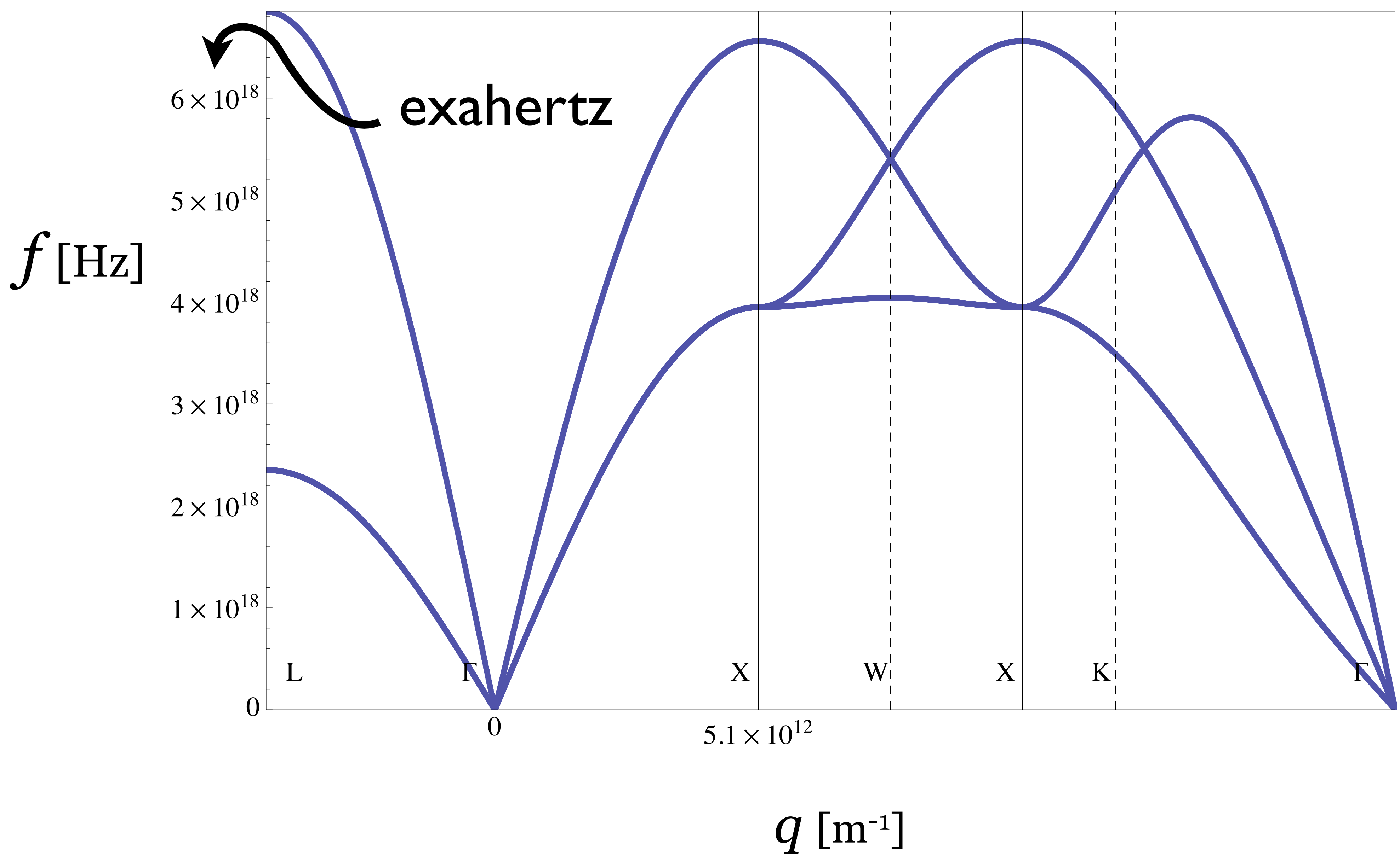
$Z_A=34, Z_C=8$

$\mu_{perovskite}/\mu_{fcc} > 1$

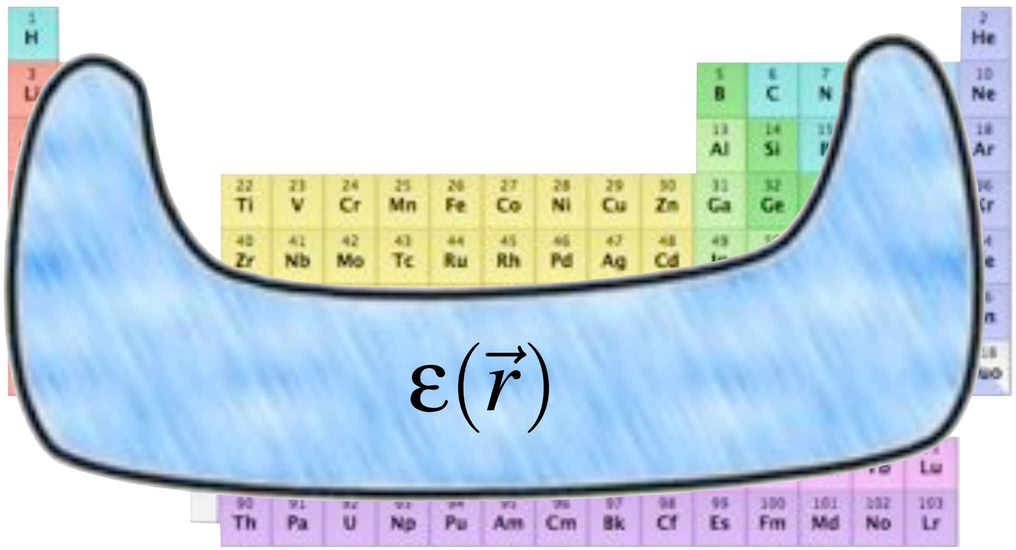
$\mu_{perovskite}/\mu_{fcc} < 1$

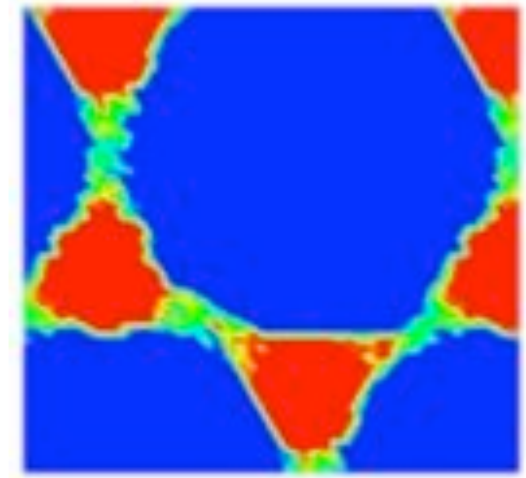
(A uniform electron gas is assumed in the calculation of the kinetic energy.)

Phonon dispersion for Z=34 fcc lattice at 10^{20} bar, ρ=4×10^{8} g/cm^3



Photonic crystals are continuous
The periodic table is discrete





Optimize a figure of merit: $F(\omega_1, \ldots \omega_n)$

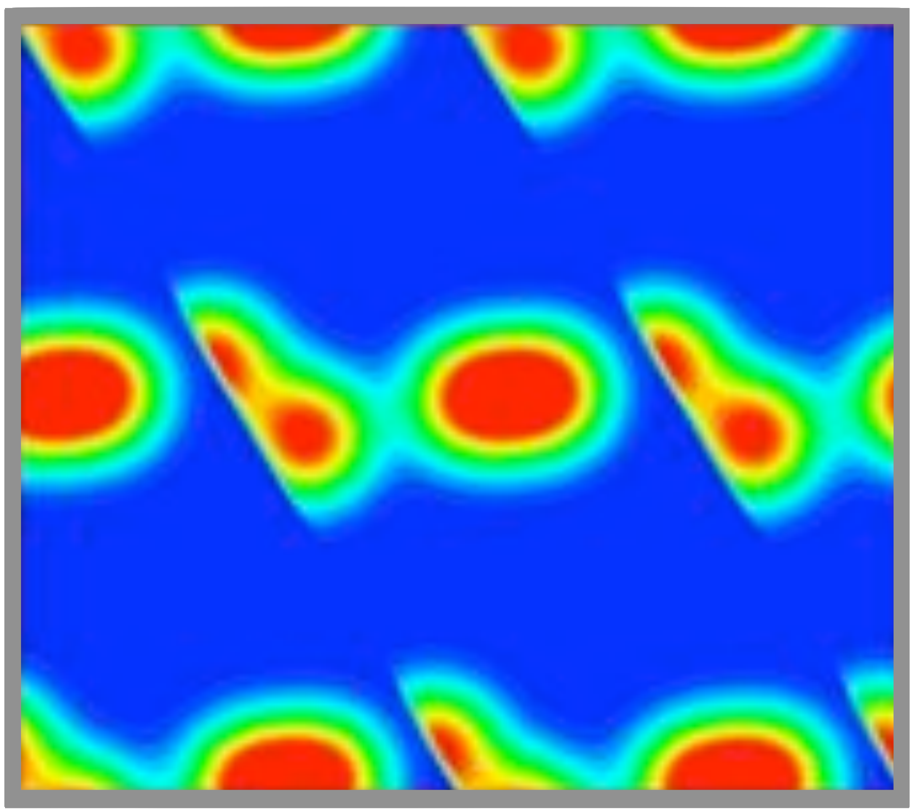
Guided by a gradient: $$\frac{\delta F(\omega_1, \ldots \omega_n)}{\delta \varepsilon(\vec{r})}$$

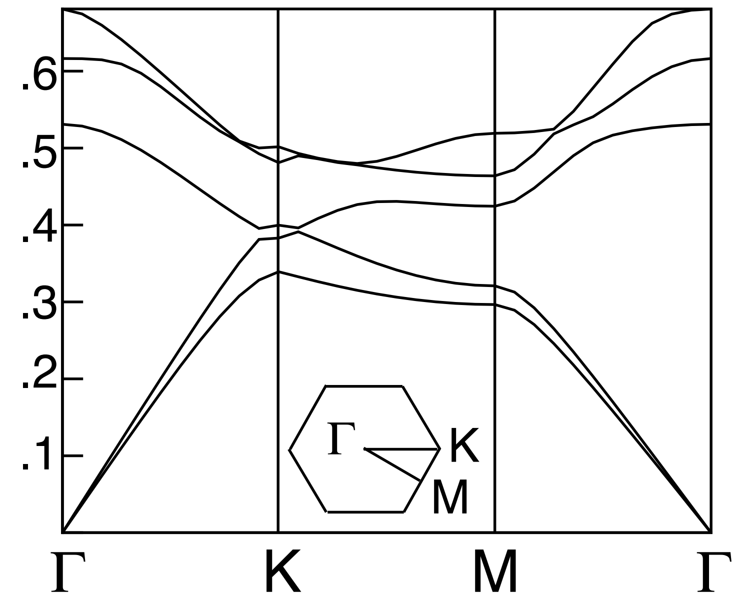
From perturbation theory: $$\frac{\delta \omega^2_{n,k}}{\omega^2_{n,k}} = \frac{\langle D_i^{(n,k)} \mid \delta \varepsilon^{-1}_{i,j} D_j^{(n,k)} \rangle}{\langle D_i^{(n,k)} \mid \varepsilon^{-1}_{i,j} D_j^{(n,k)} \rangle}$$

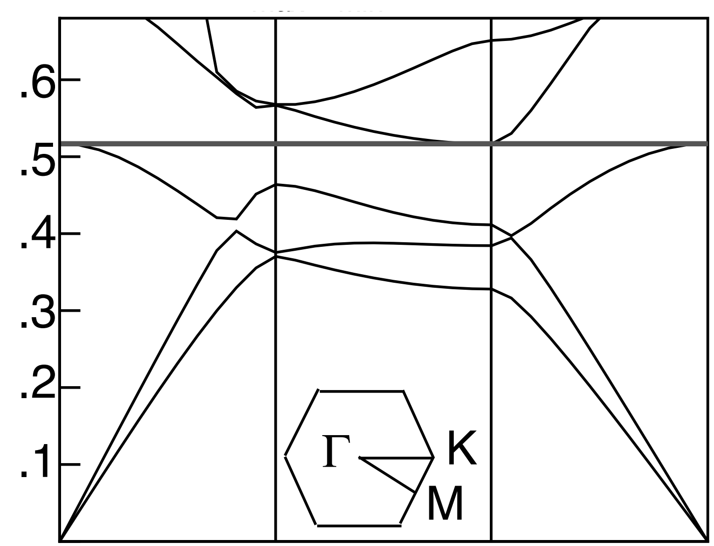
Bao & Dobson, Surv. Math. Ind. **8**, 37 (1998); Cox & Dobson, J. Appl. Math. **59**, 2108 (1999); Qiu & He, Opt. Soc. Am. B **17**, 1027 (2000); Shen, Ye & He, PRB **68**, 35109 (2003); Chen, Sharkway, Shi & Prather, Opt. Exp. **11**, 317 (2003)

Optimizing bandgap at fixed dielectric contrast on a triangular lattice

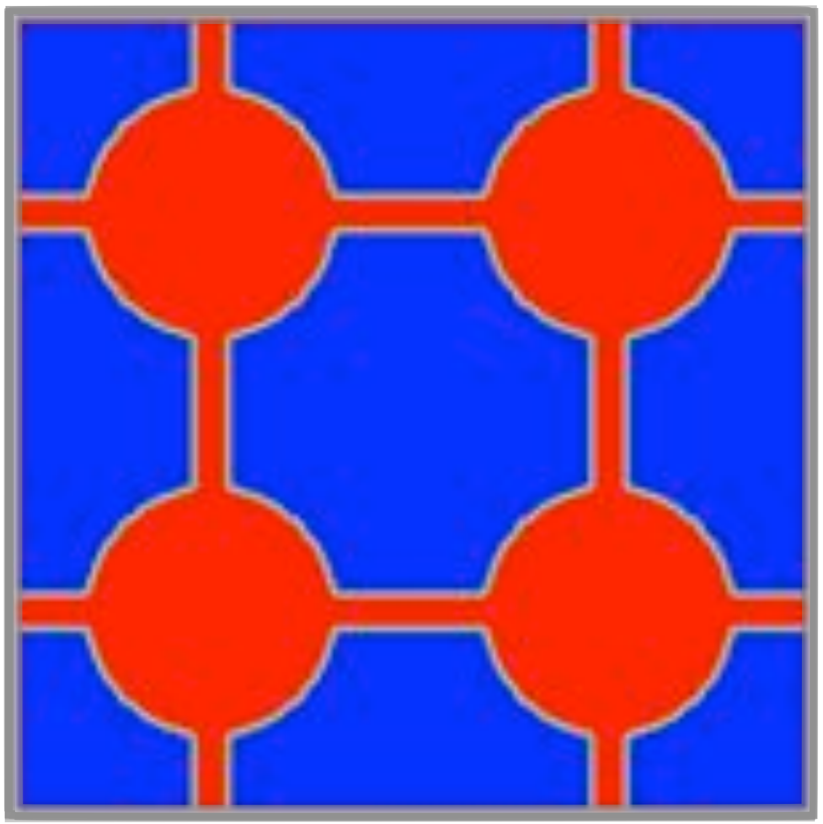
$\varepsilon_{max}/\varepsilon_{min}=6.9$

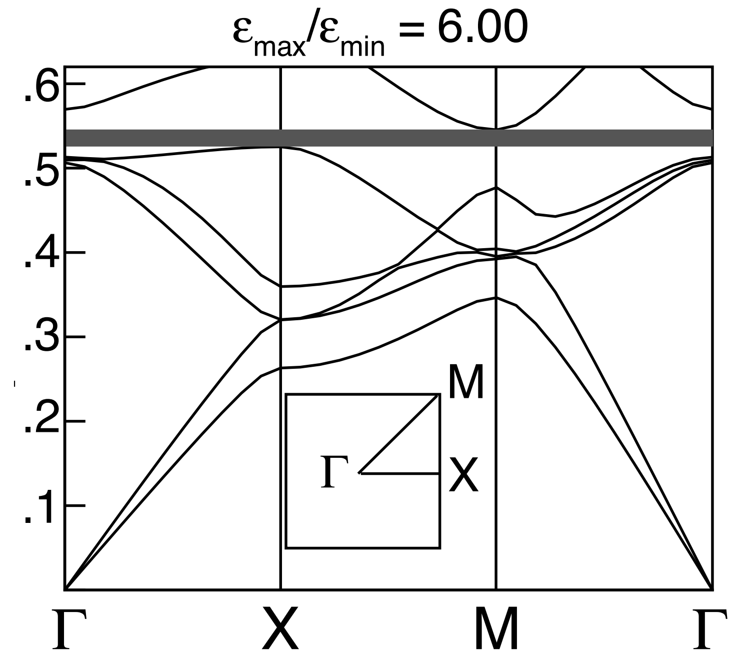


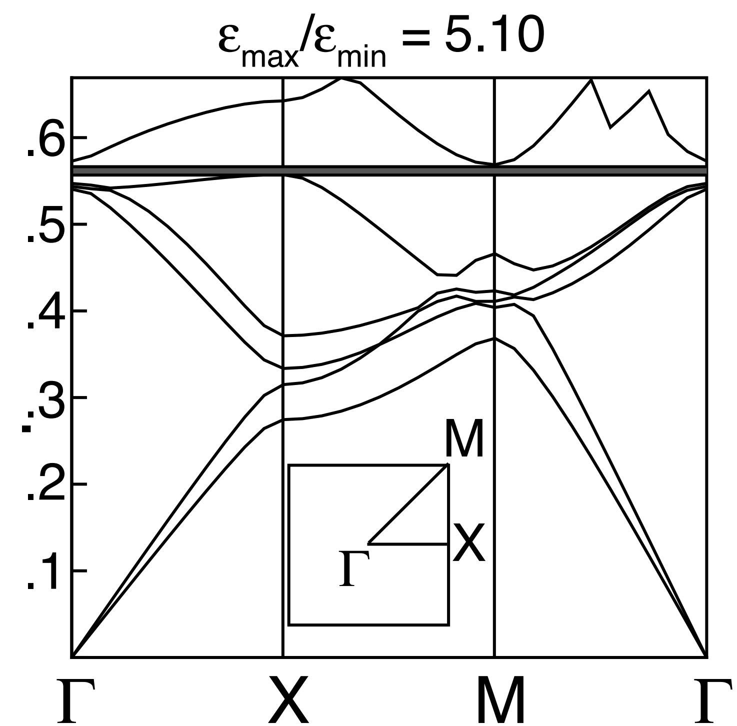


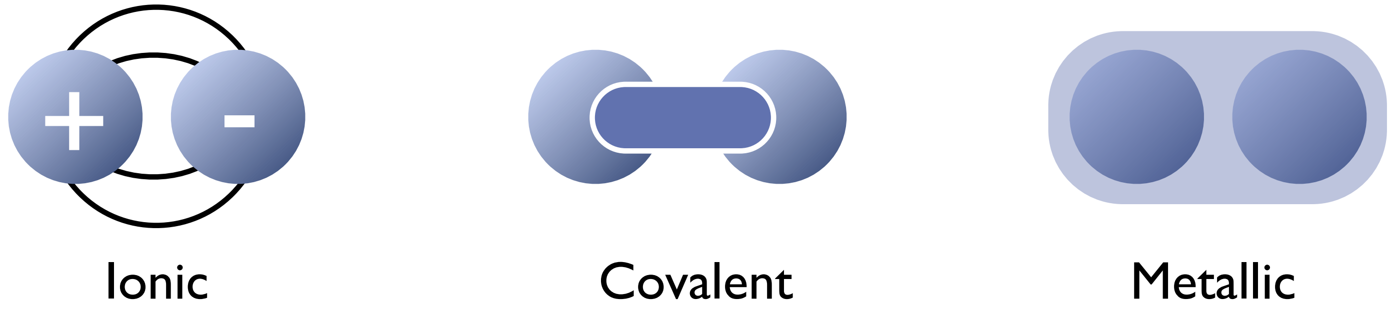


Optimize for a full gap at minimal dielectric contrast on a square lattice

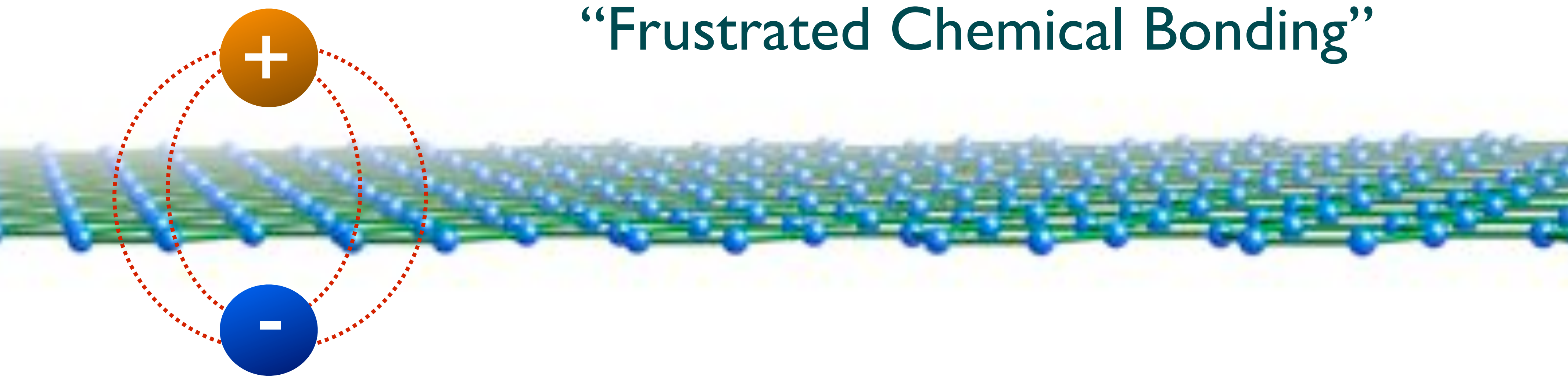




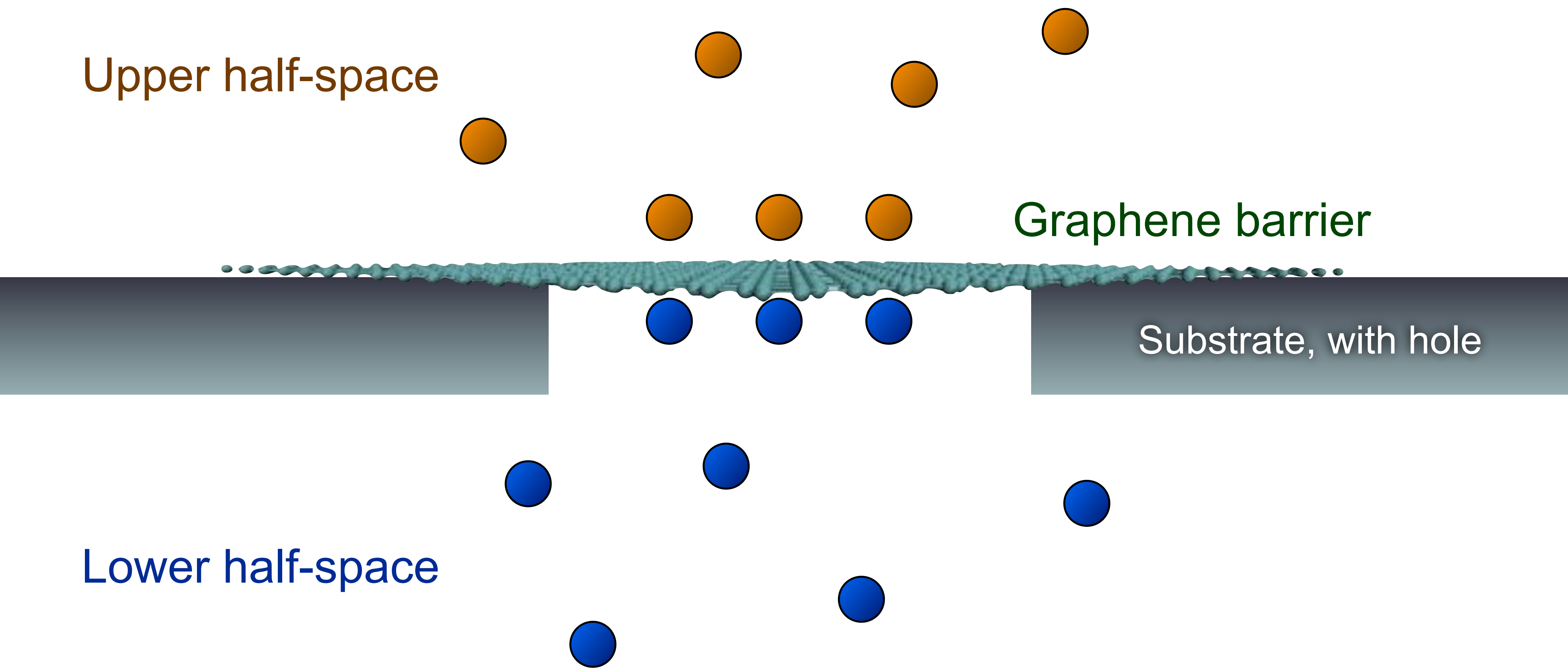


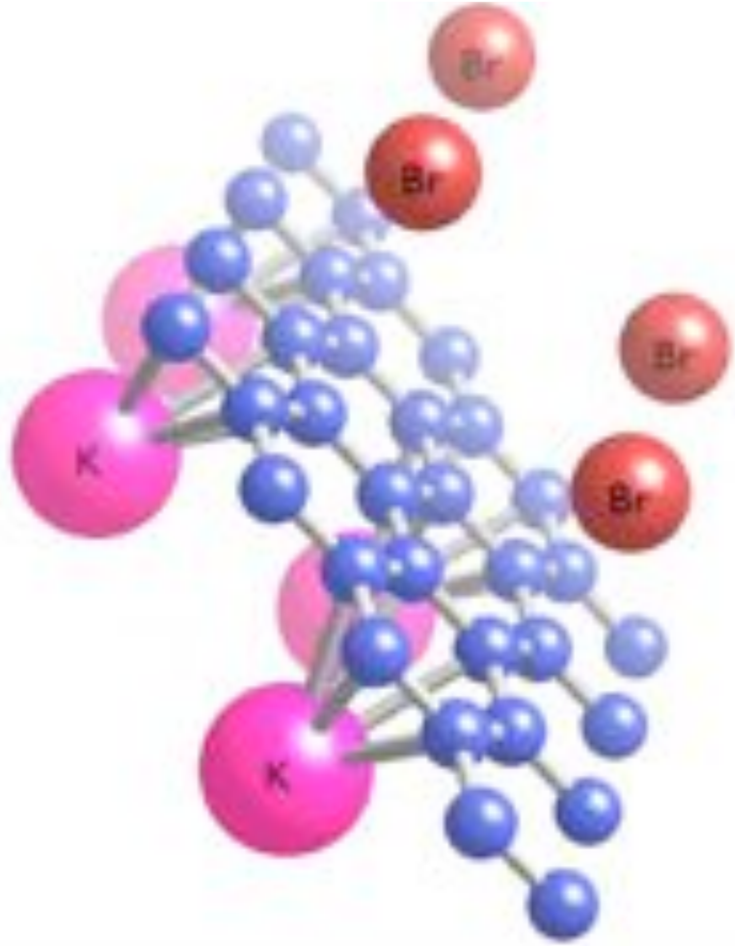


"Frustrated Chemical Bonding"



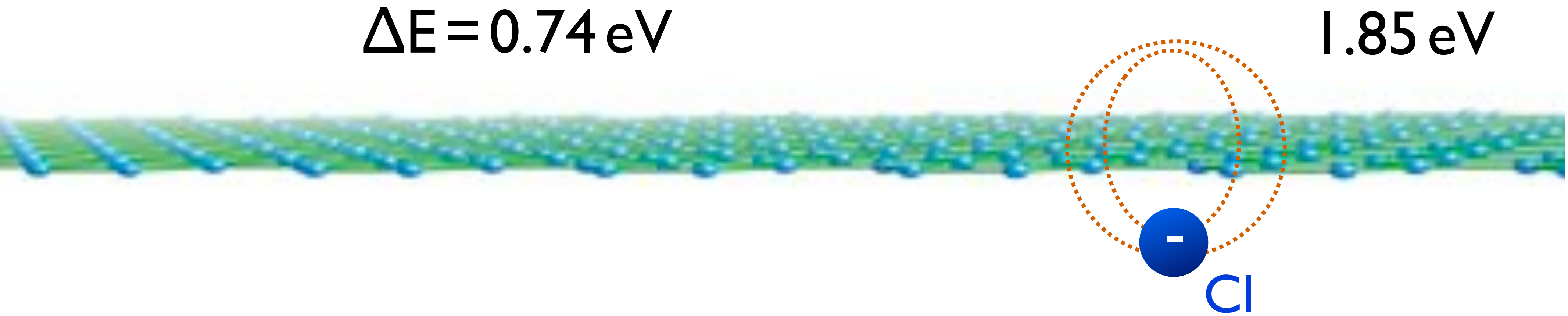
A chemical bond is defined not only by the atoms doing the binding, but also by the background space in which they bind.


Upper half-space
Graphene barrier
Substrate, with hole
Lower half-space



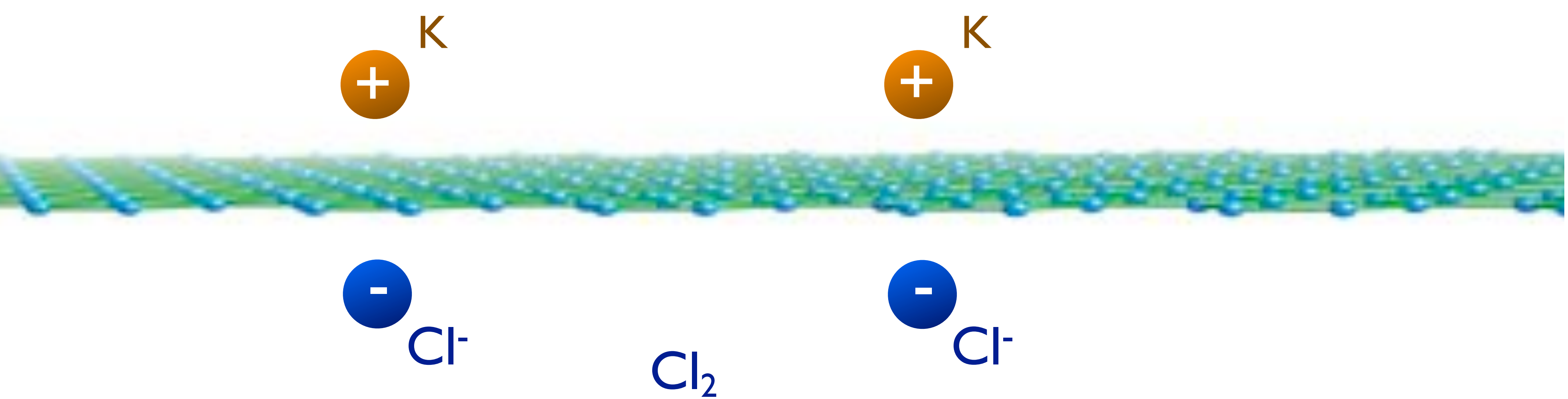
Br remains unbound covalently: we are in the desired topologically constrained regime.

Is the alkali-halogen interaction fully screened by the graphene?

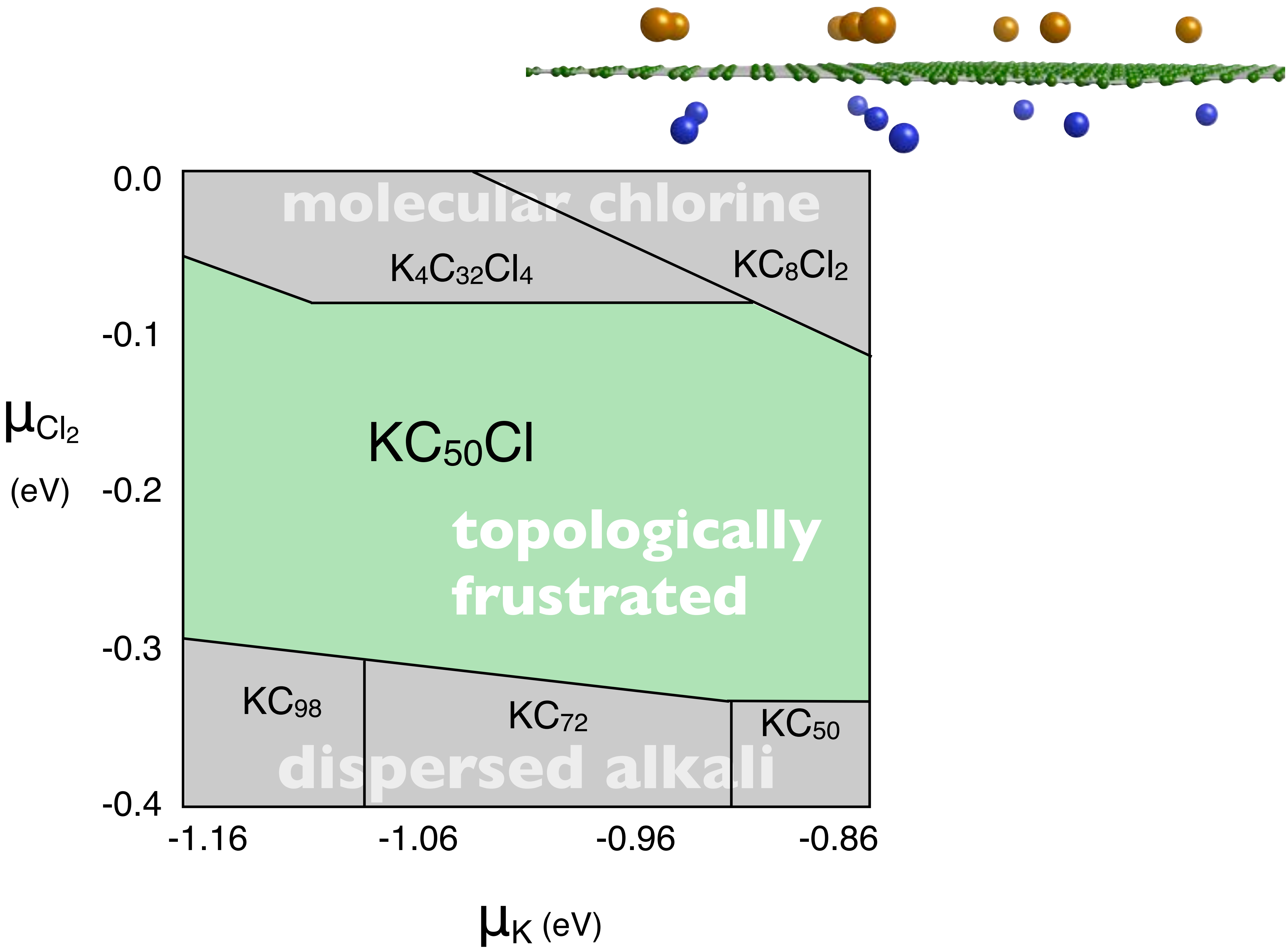


Each adatom sees the effect of the other: graphene is not a perfect conductor

What about alternative configurations of the halogens?

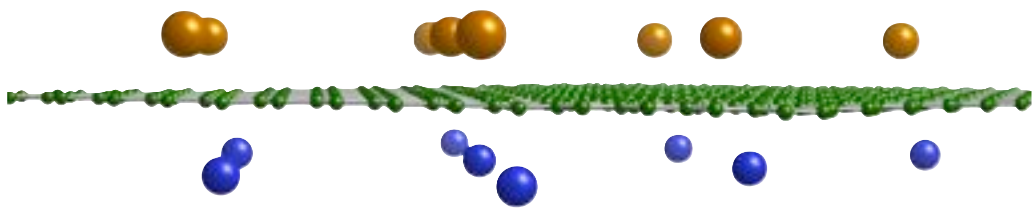


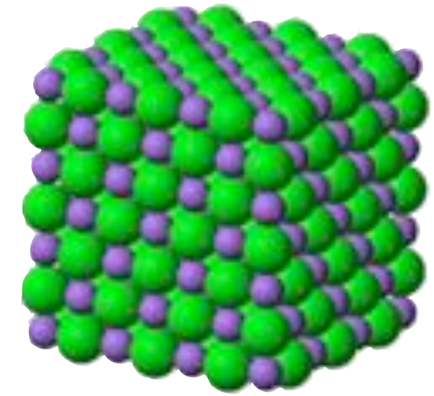
Test the phase diagram...

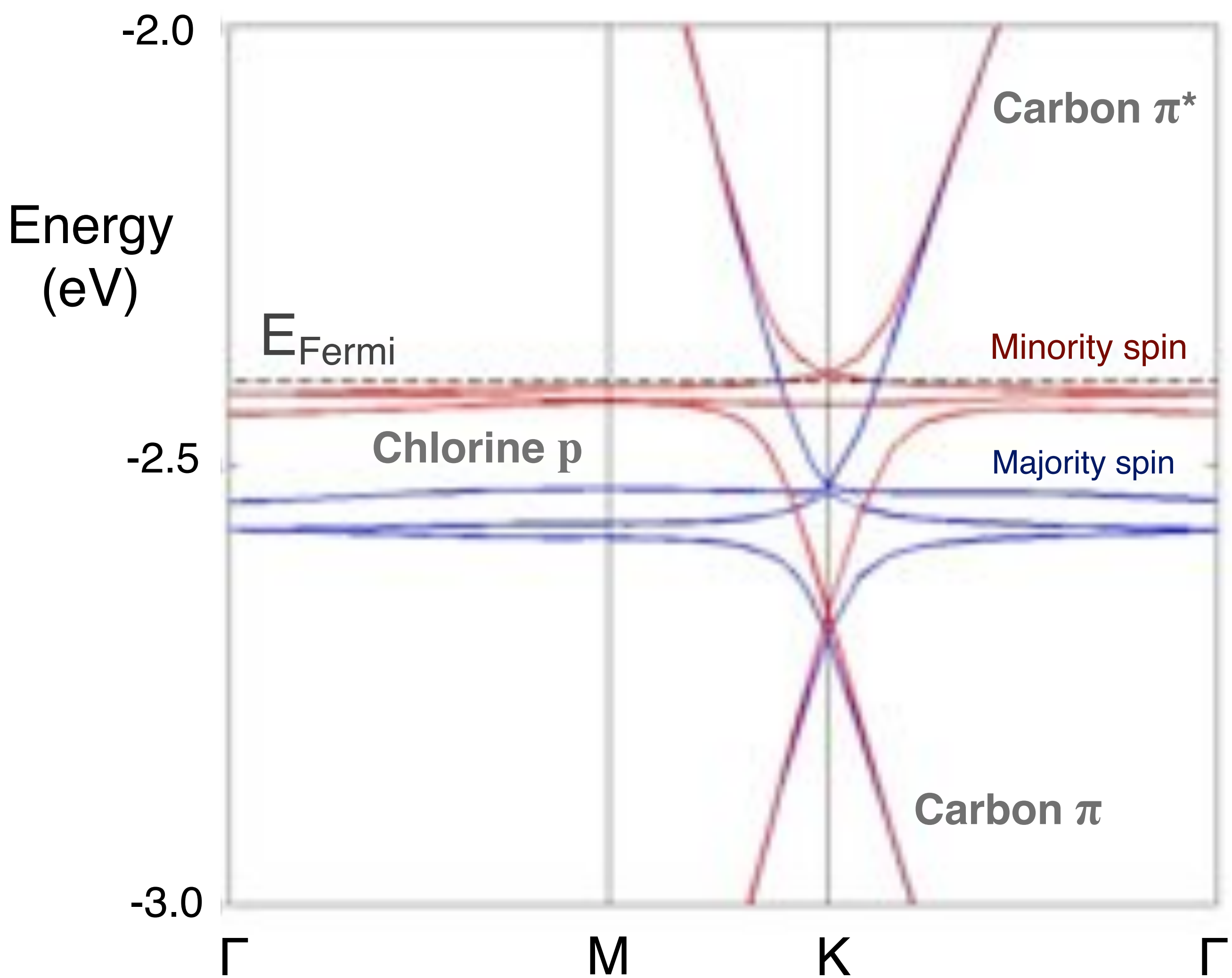


molecular chlorine
K4C32Cl4
KC8Cl2
KC50Cl
topologically frustrated
KC98
KC72
KC50
dispersed alkali
μCl2 (eV)
0.0
-0.1
-0.2
-0.3
-0.4
-1.16
-1.06
-0.96
-0.86
μK (eV)

A self-organized bandstructure

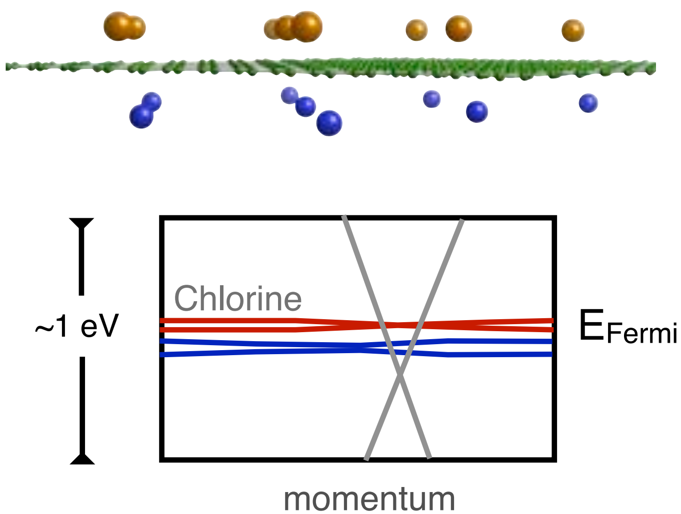


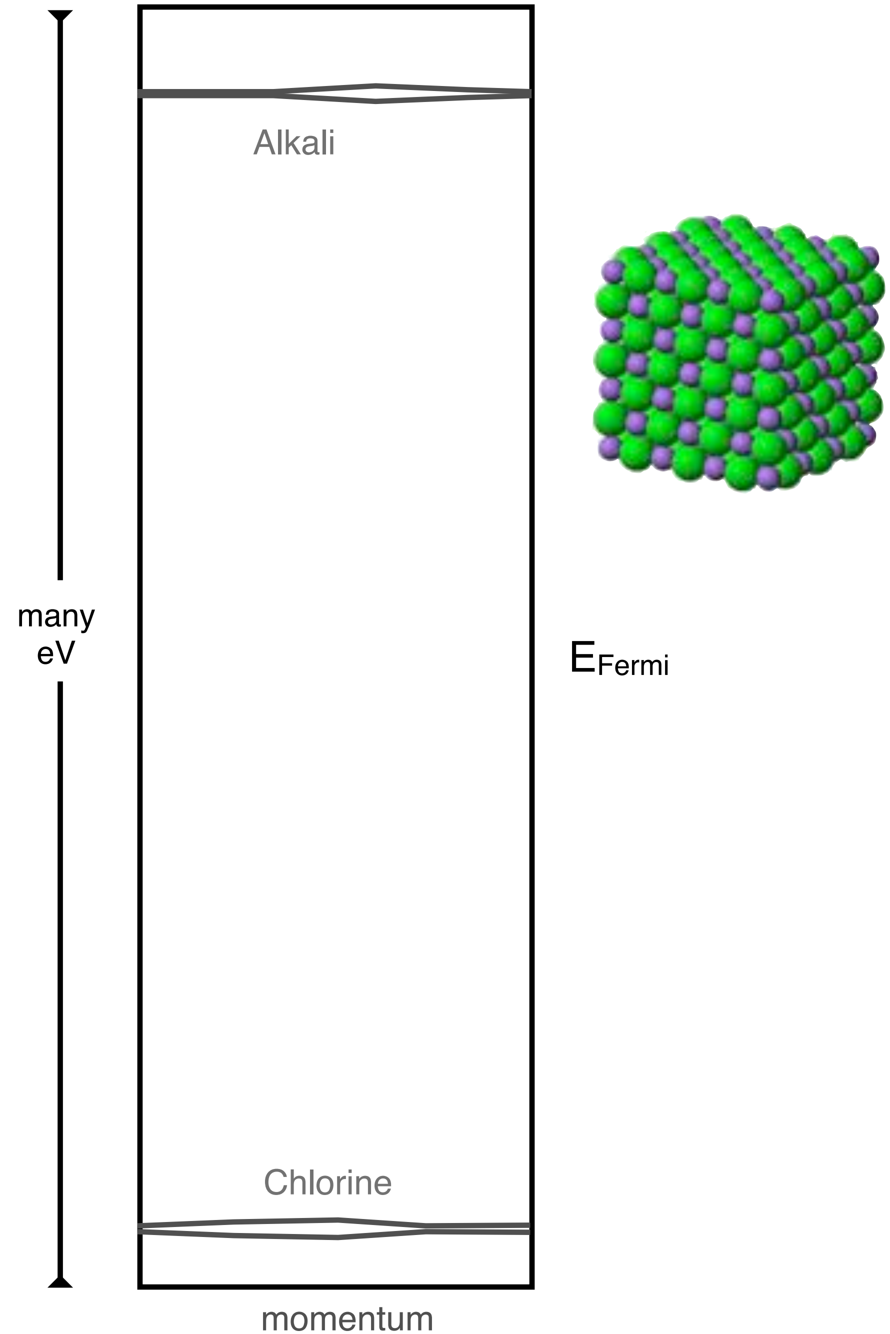




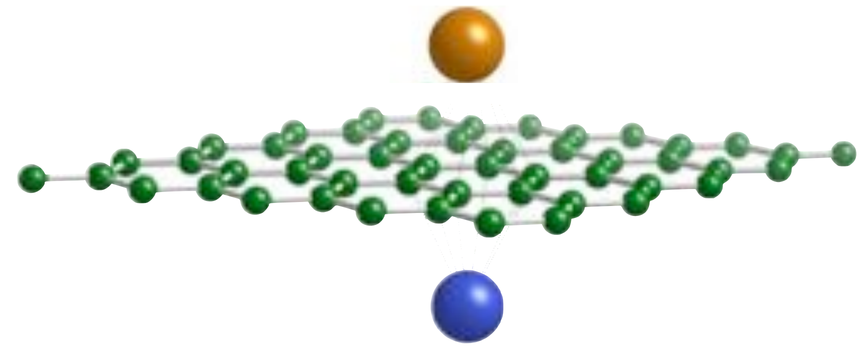
$KC_{50}Cl$

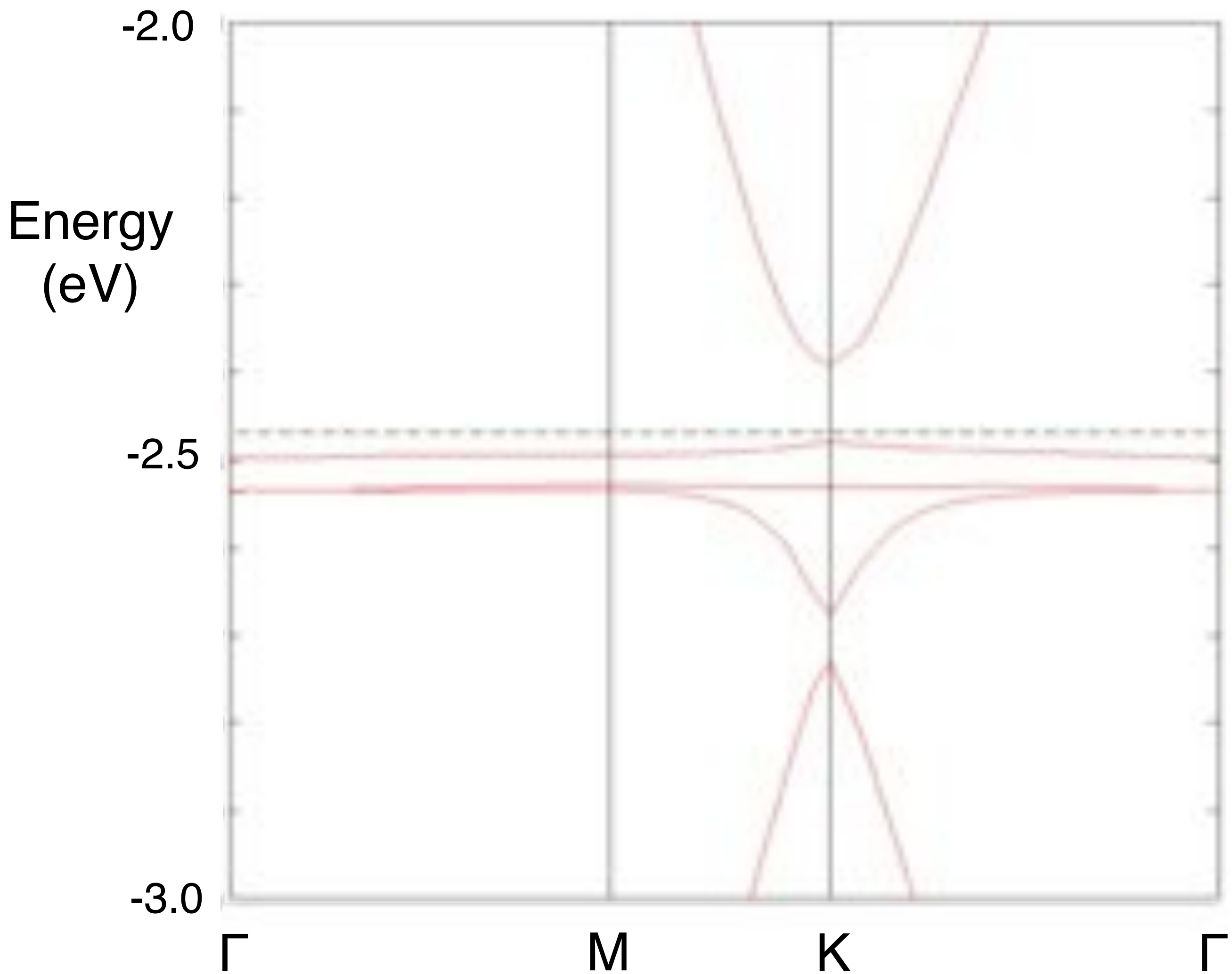
Compare frustrated & unfrustrated salt crystals:



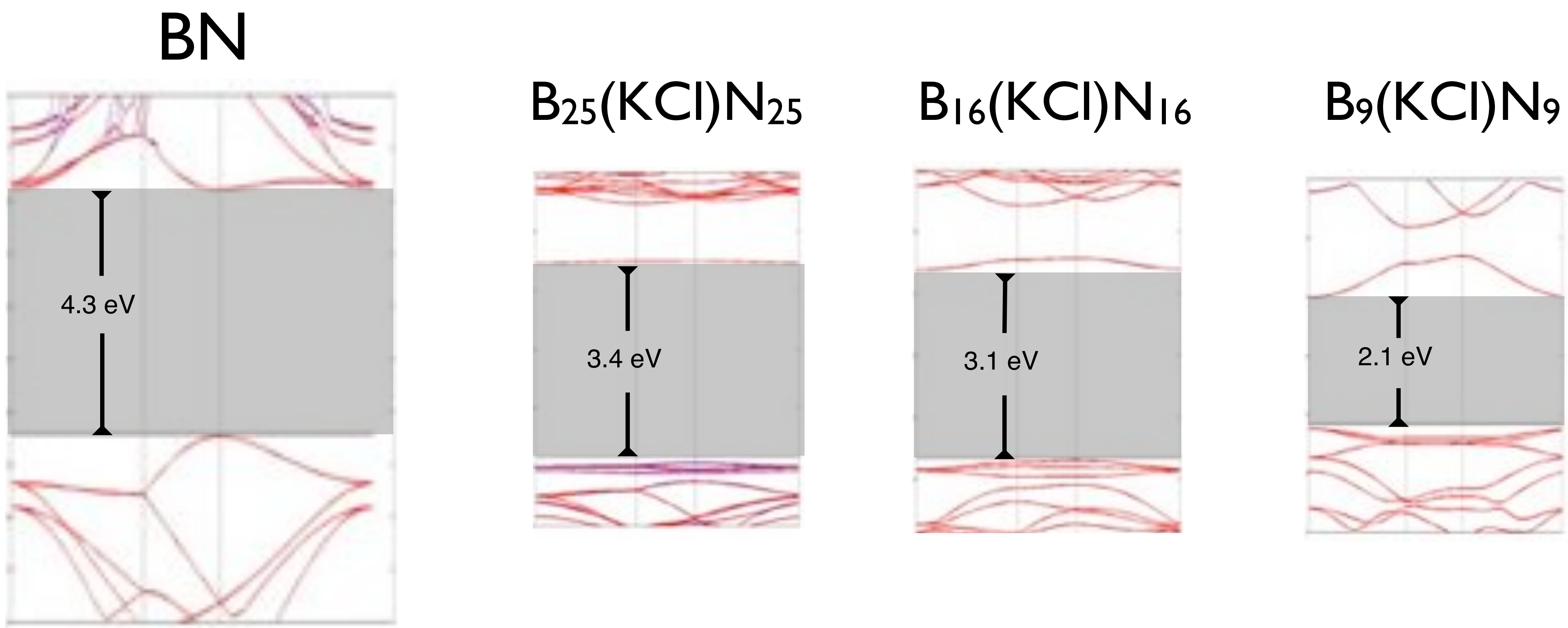


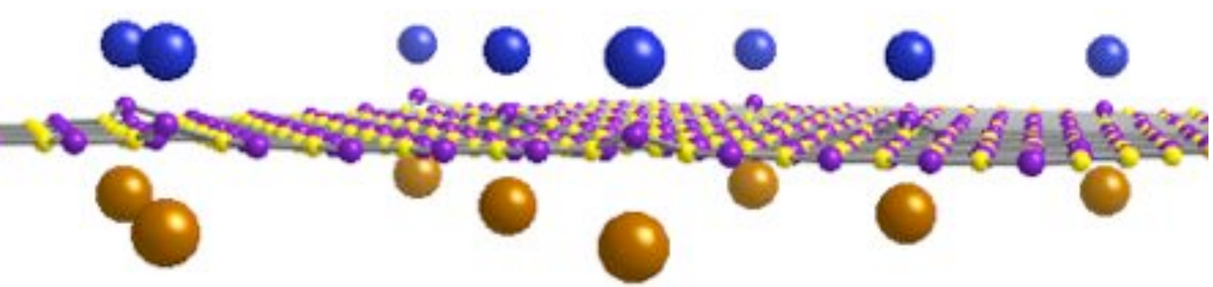
Optimize the Cl position...



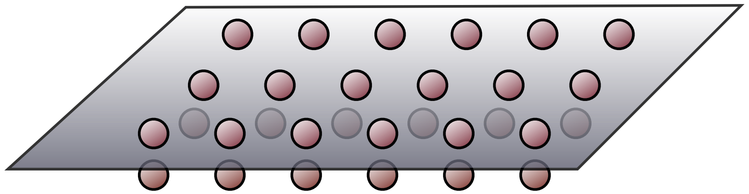


- Huge electron-phonon coupling
- Superconductor?
- Catalyst?
- Correlated states?

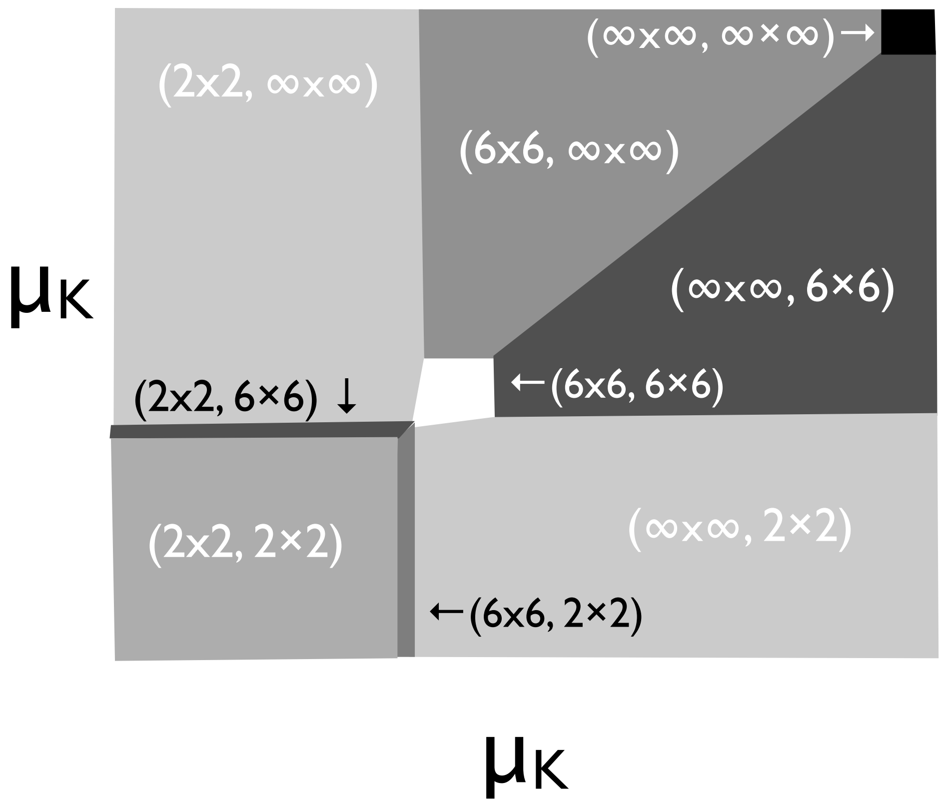


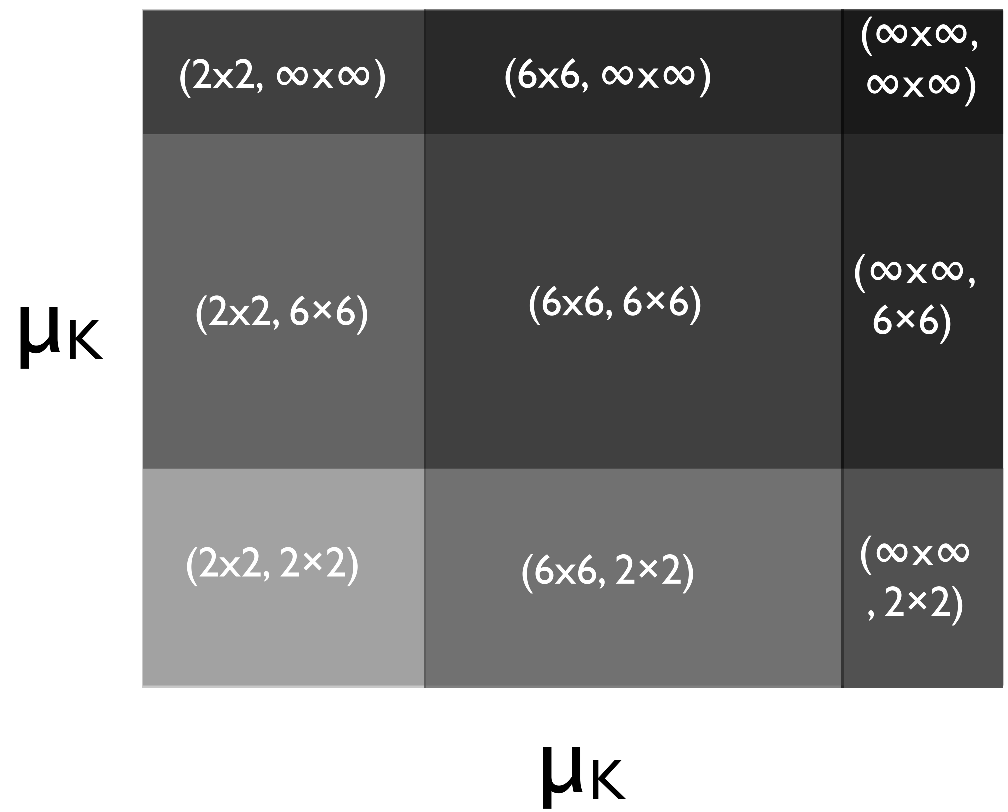


← boron nitride barrier



Non-interacting

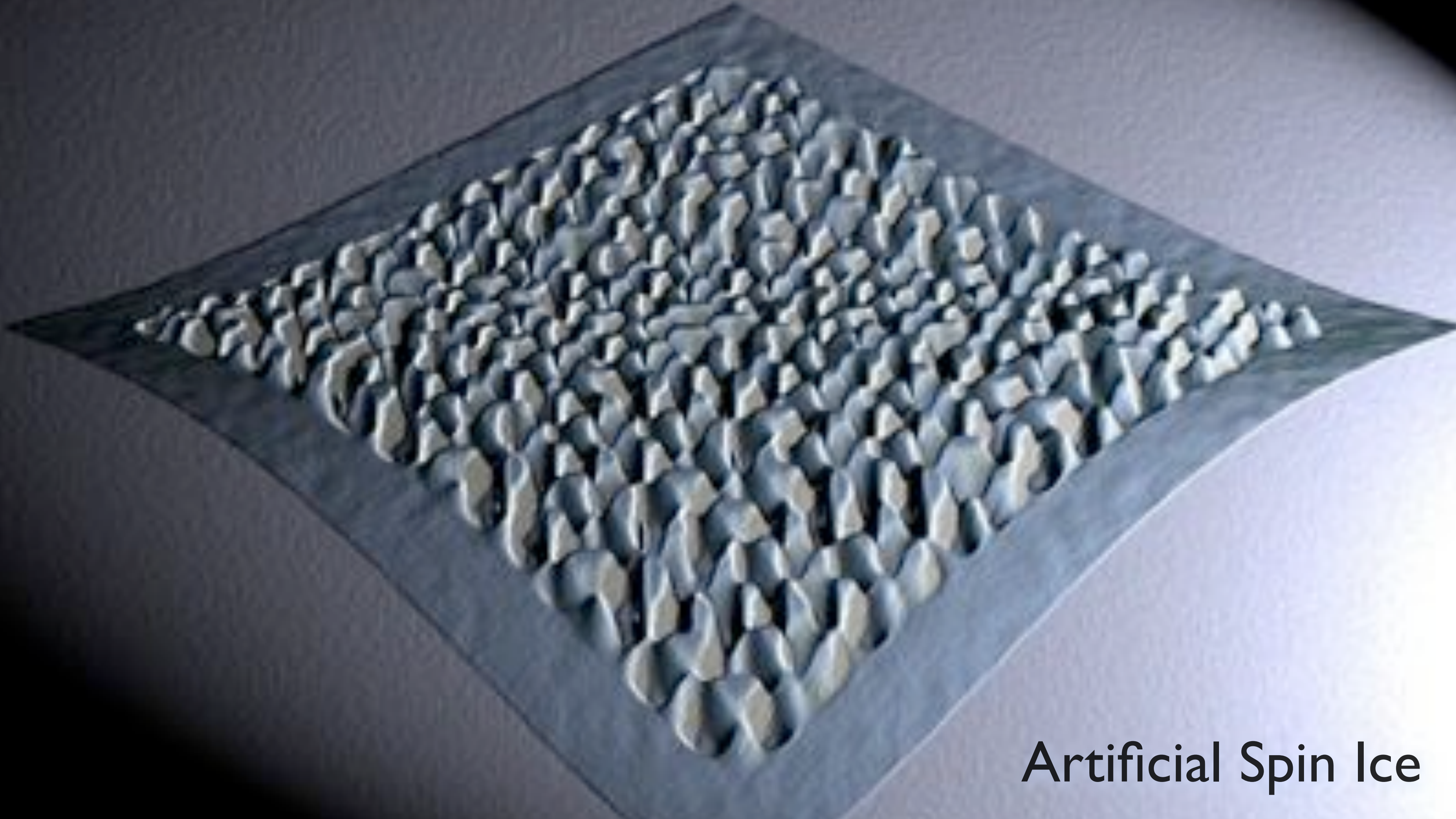




The *same thing* (K) on both sides...

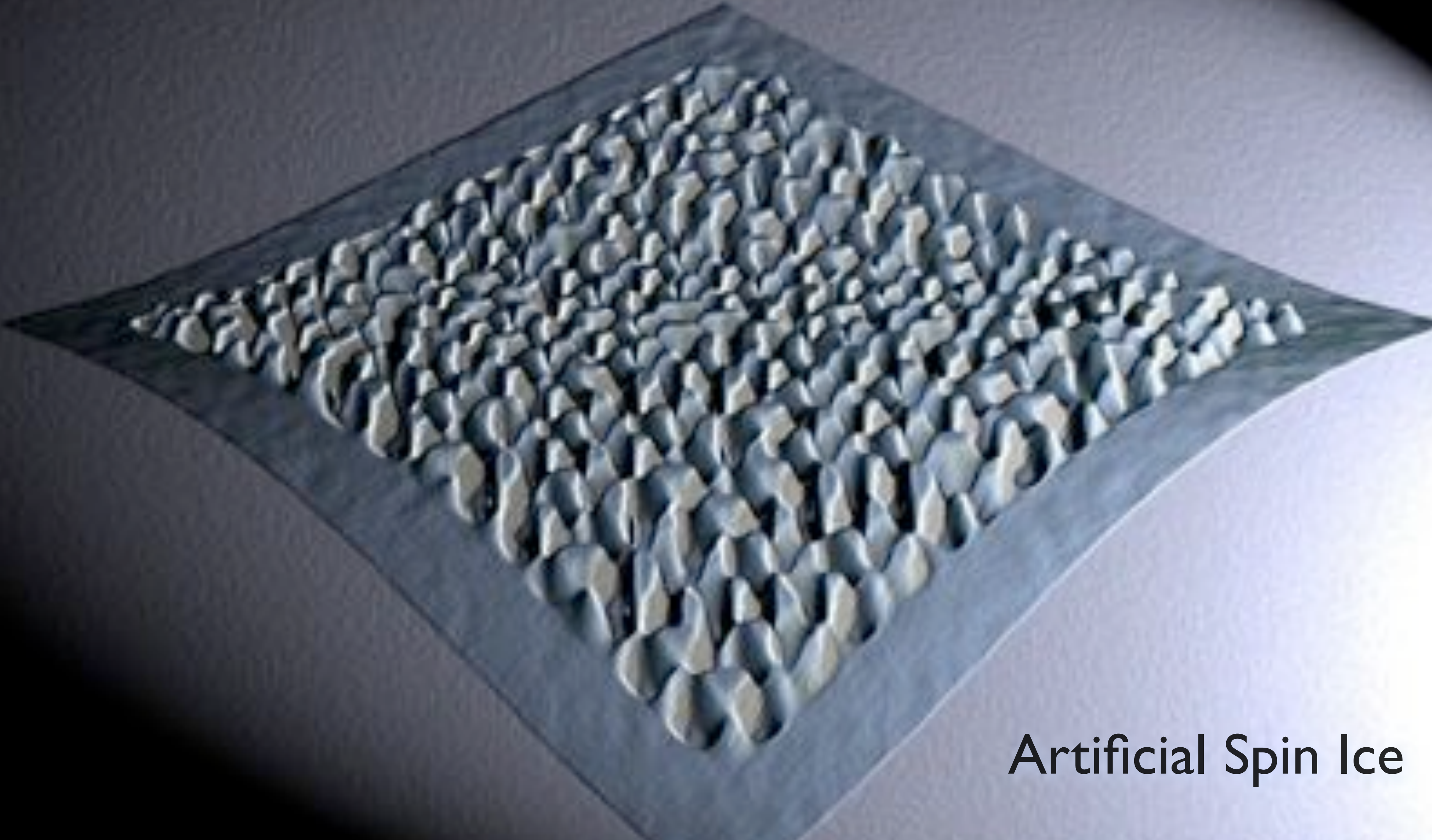
...non-monotonic $\rho(\mu)$, spontaneous symmetry breaking

Computational Experiment

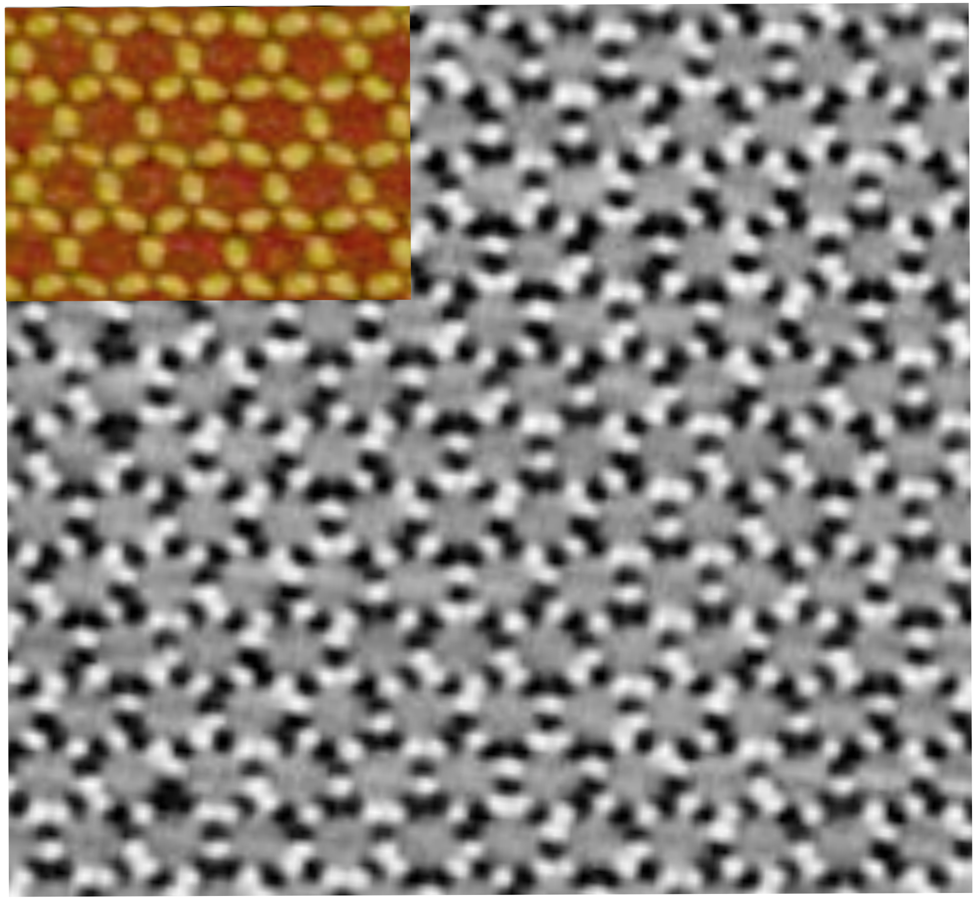


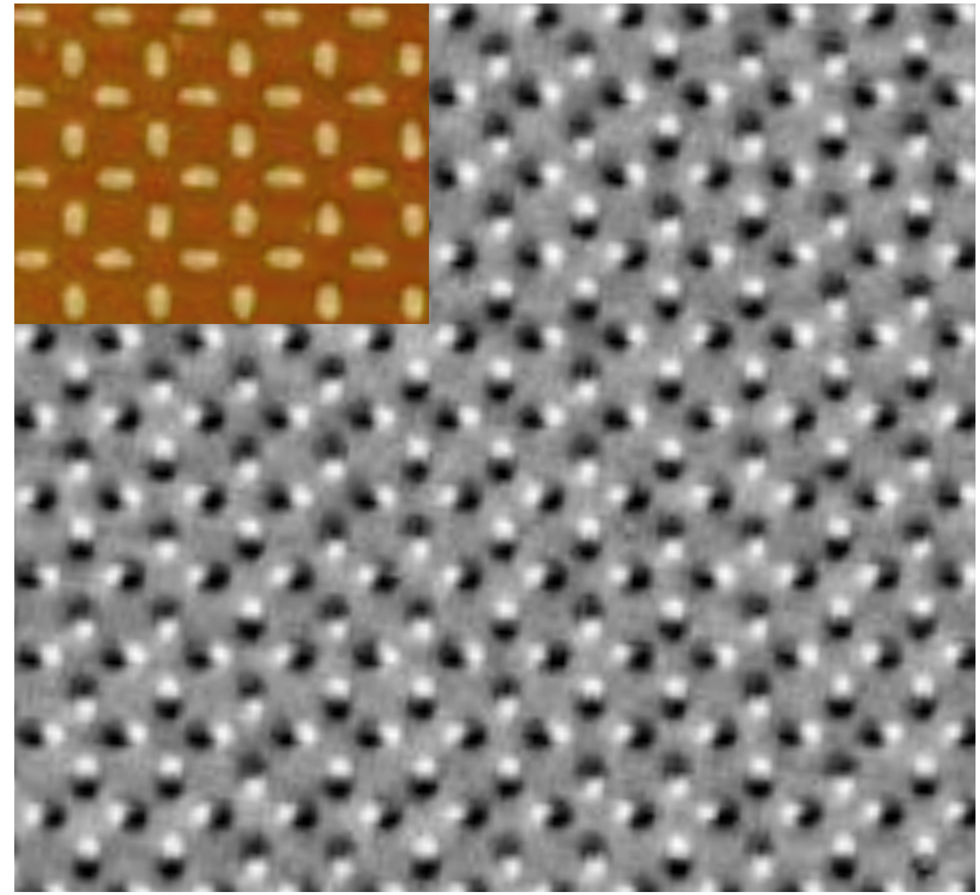
Artificial Spin Ice

Experimental computation



Artificial Spin Ice

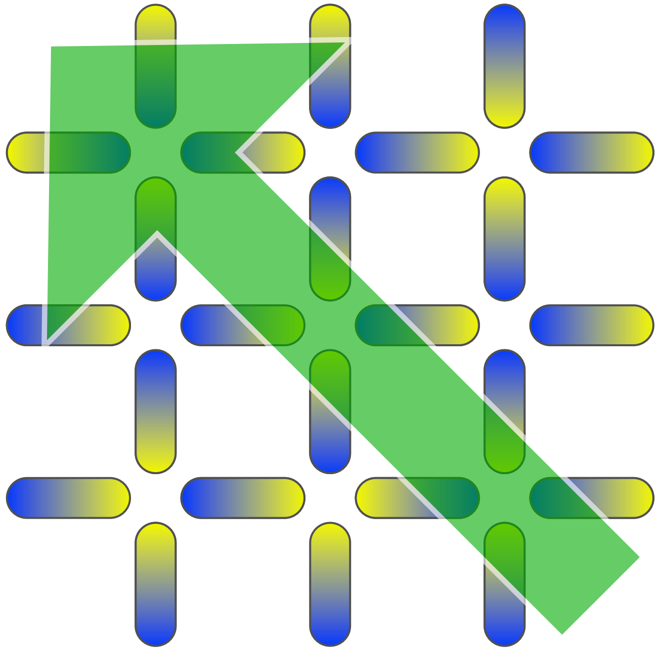




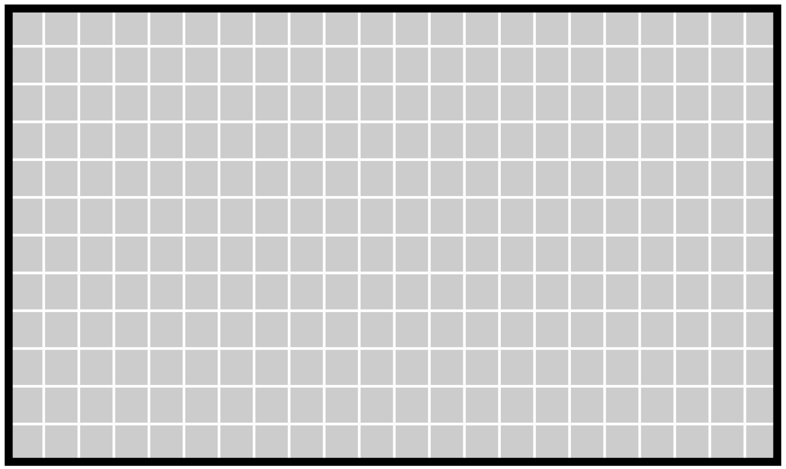
Magnetic islands small enough to be single-domain, arrayed on a lattice: an experimental Ising model with all degrees of freedom exposed.

R. Wang, C. Nisoli, R. S. Freitas, J. Li, W. McConville, B. Cooley, M. S. Lund, N. Samarth, C. Leighton, V. H. Crespi & P. Schiffer, Nature **439**, 303 (2006)

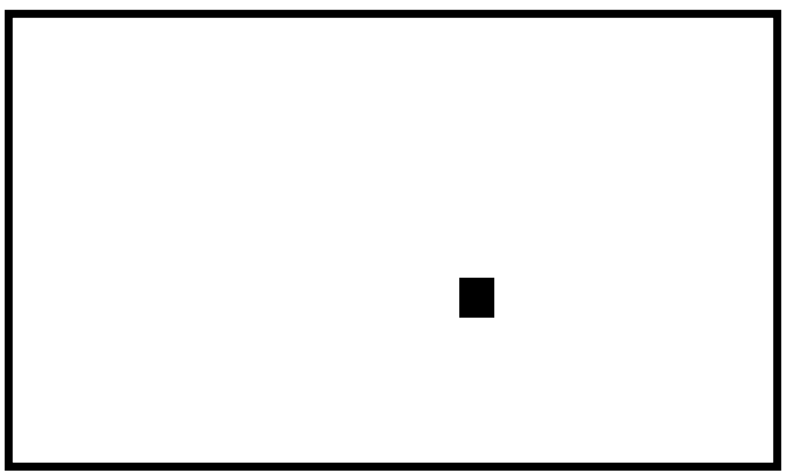
“Anneal” the system with a rotating, shrinking external magnetic field.



Entropy as information



$$-\sum_{i=1}^{N} p_i \log p_i$$

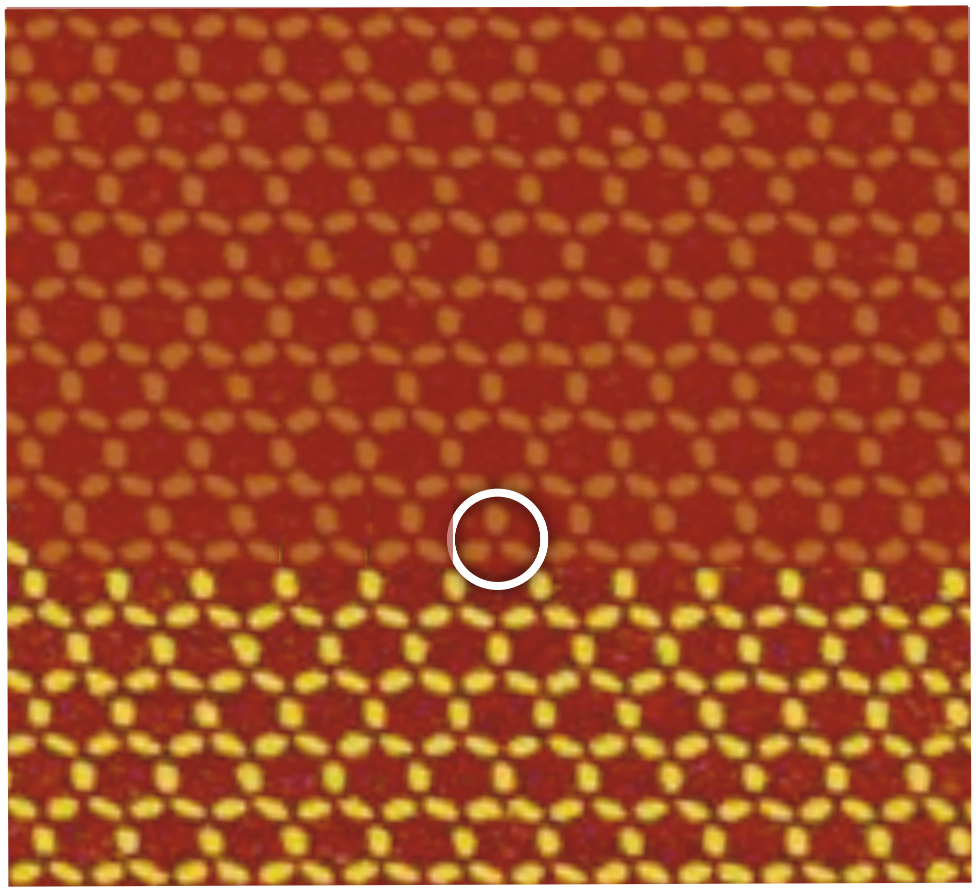


$$-\sum_{i=1}^{N} \frac{1}{N} \log \frac{1}{N}$$

$$= -\log \frac{1}{N} \quad = \log N$$

The entropy of the initial macrostate is the information gained in learning the actual microstate.

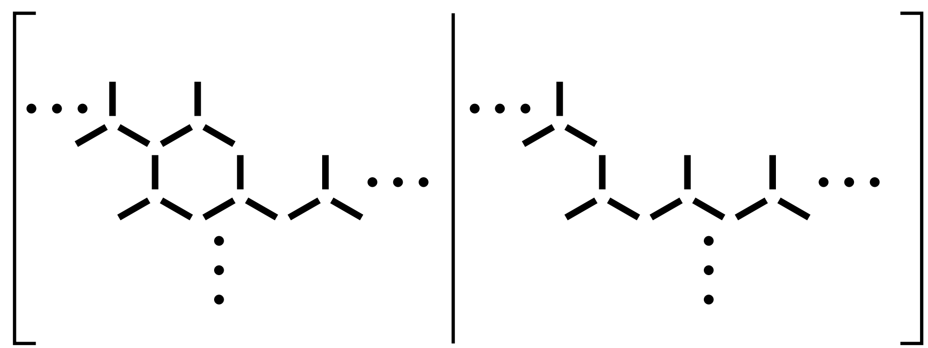
Reveal our microstate bit by bit...

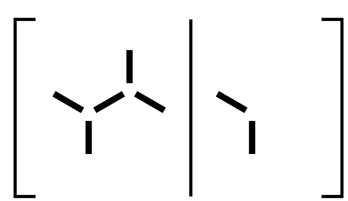


The entropy per island is one third of the information gained by learning the states of these three sites.

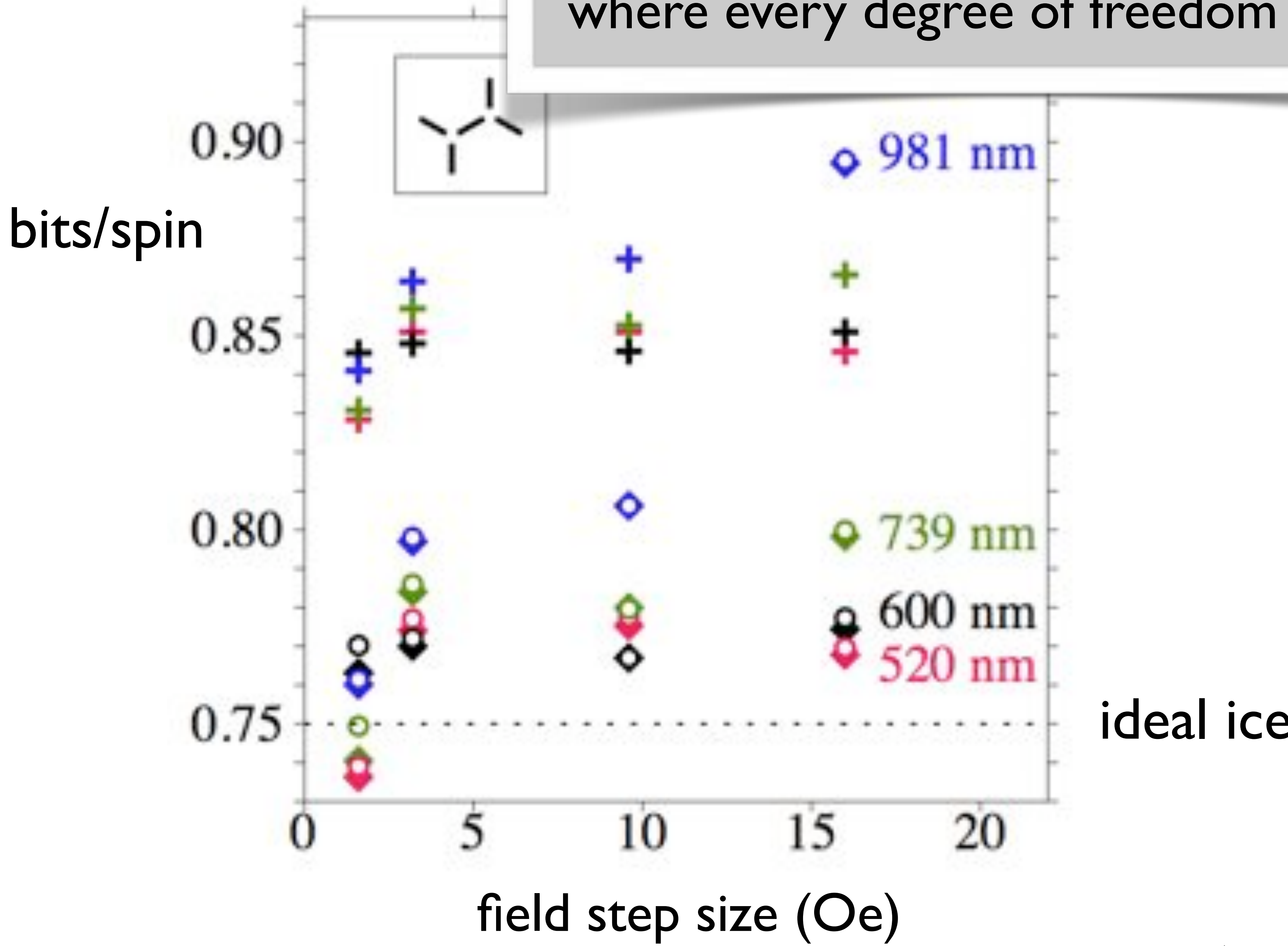
The total entropy can be built up as a summation of conditional entropies

$$S(\Lambda \cup \Gamma) = S(\Lambda|\Gamma) + S(\Gamma)$$

$3s = S$ 

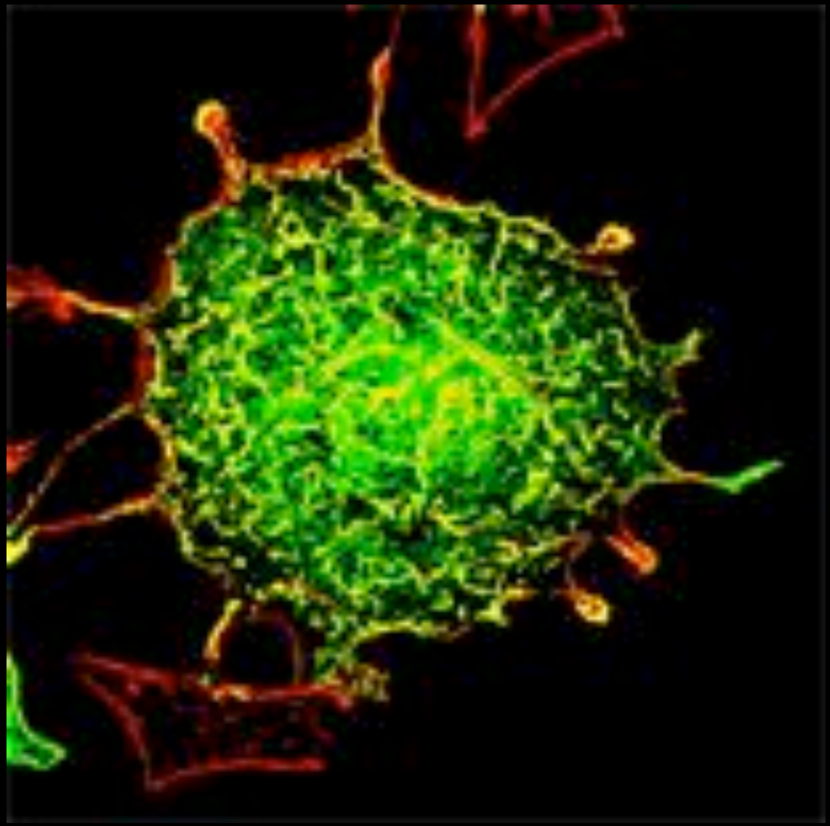
$3s \leq S$ 

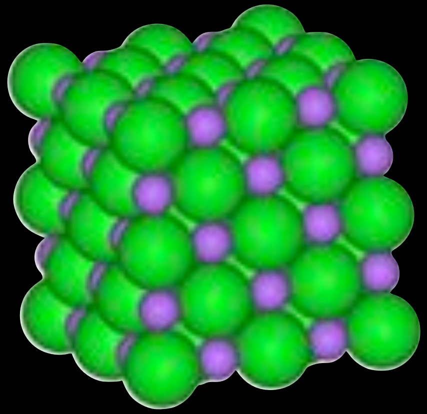
measure entropy without measuring heat: extract it as if from a simulation where every degree of freedom is visible



Lammert et al, Nature Physics, (2010)

manifold of low-lying
metastable states





ground state

Homeostasis

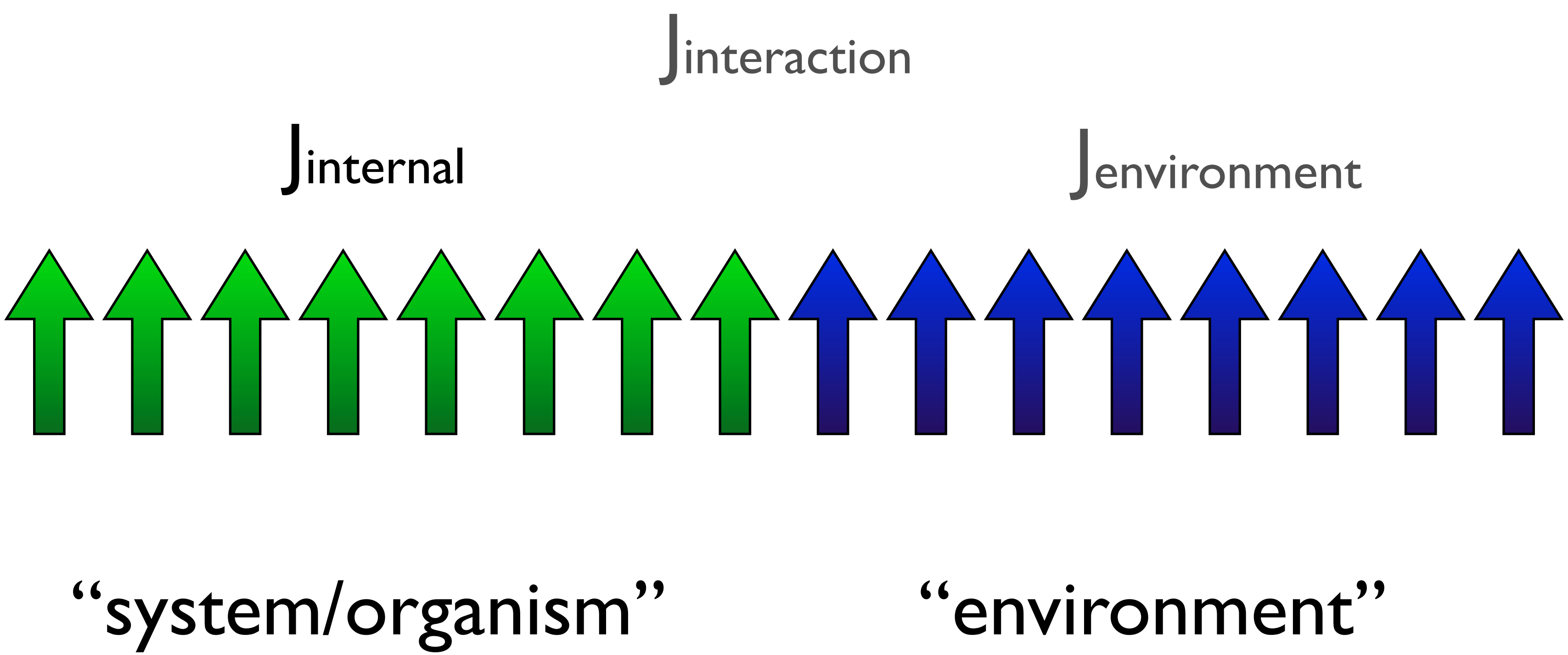
minimize the mutual information between a system and its environment

$$I(X,Y)=\sum_{x\in X}\sum_{y\in Y}p(x,y)\log\left(\frac{p(x,y)}{p(x)\,p(y)}\right)$$

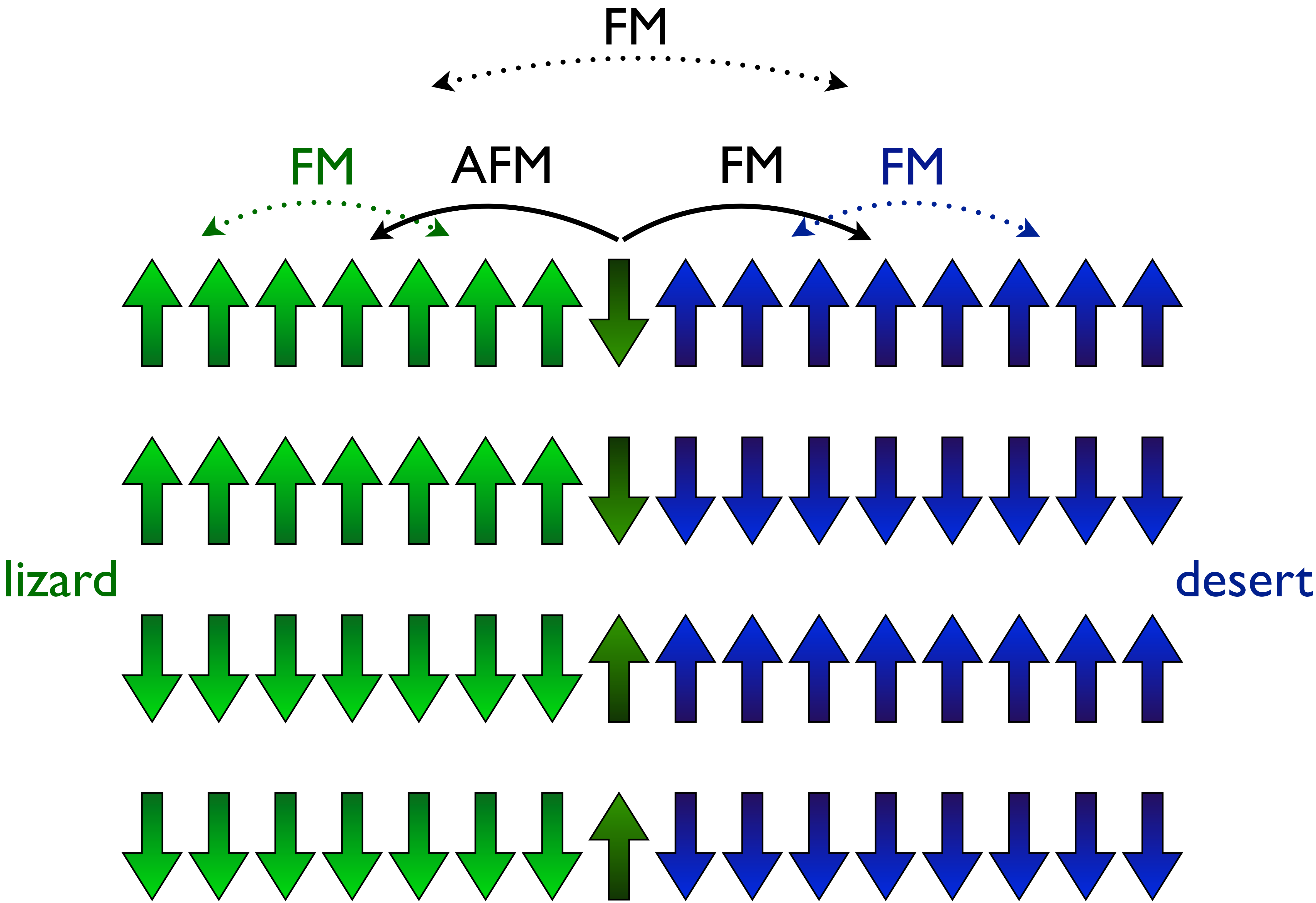
$$E = \sum H_i s_i + \sum J_{ij} s_i s_j$$

$$J_{ij} = S_{ij} \, \mathrm{e}^{-\lambda |i-j|}$$

$$|S_{ij}| < C$$

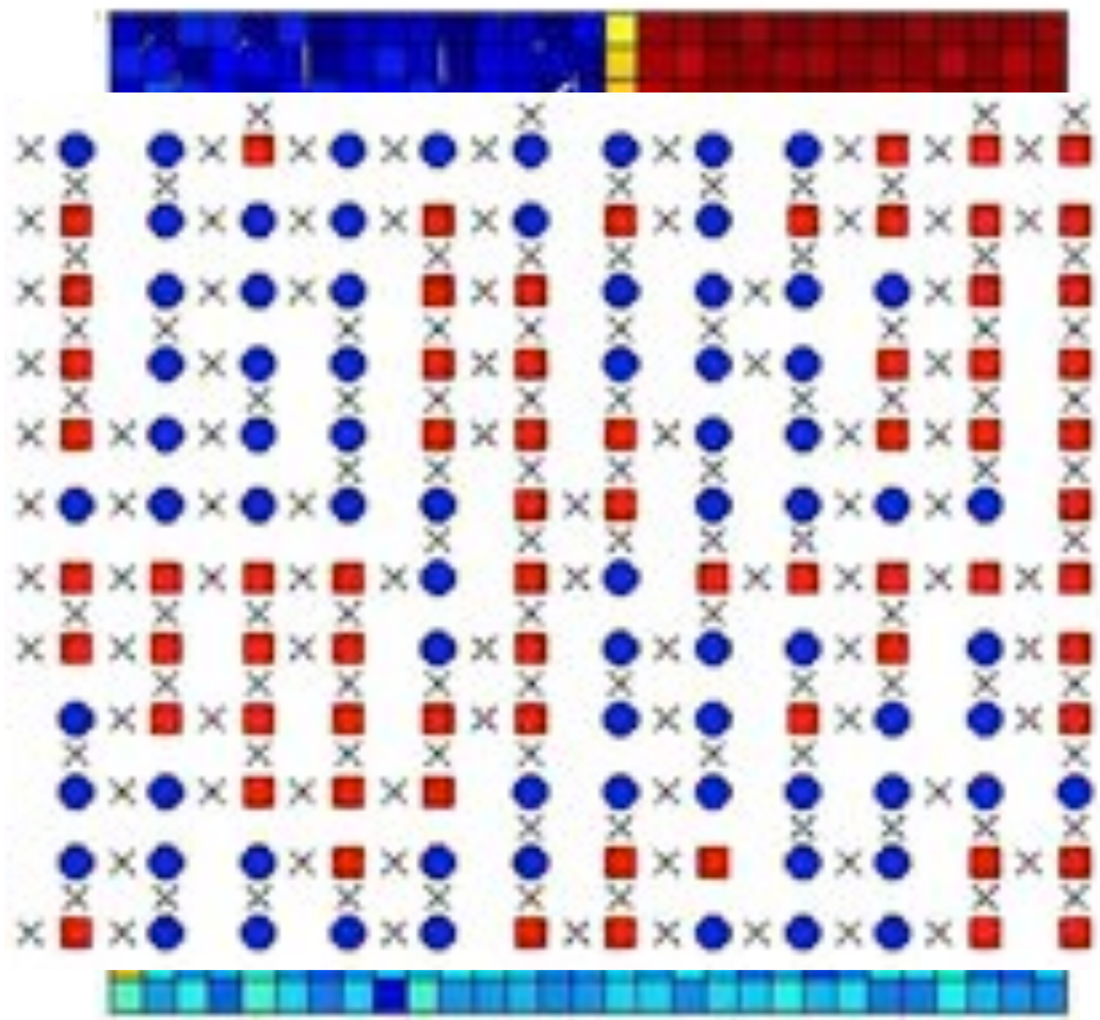


The system has to “spend” a bit to encode its environment.

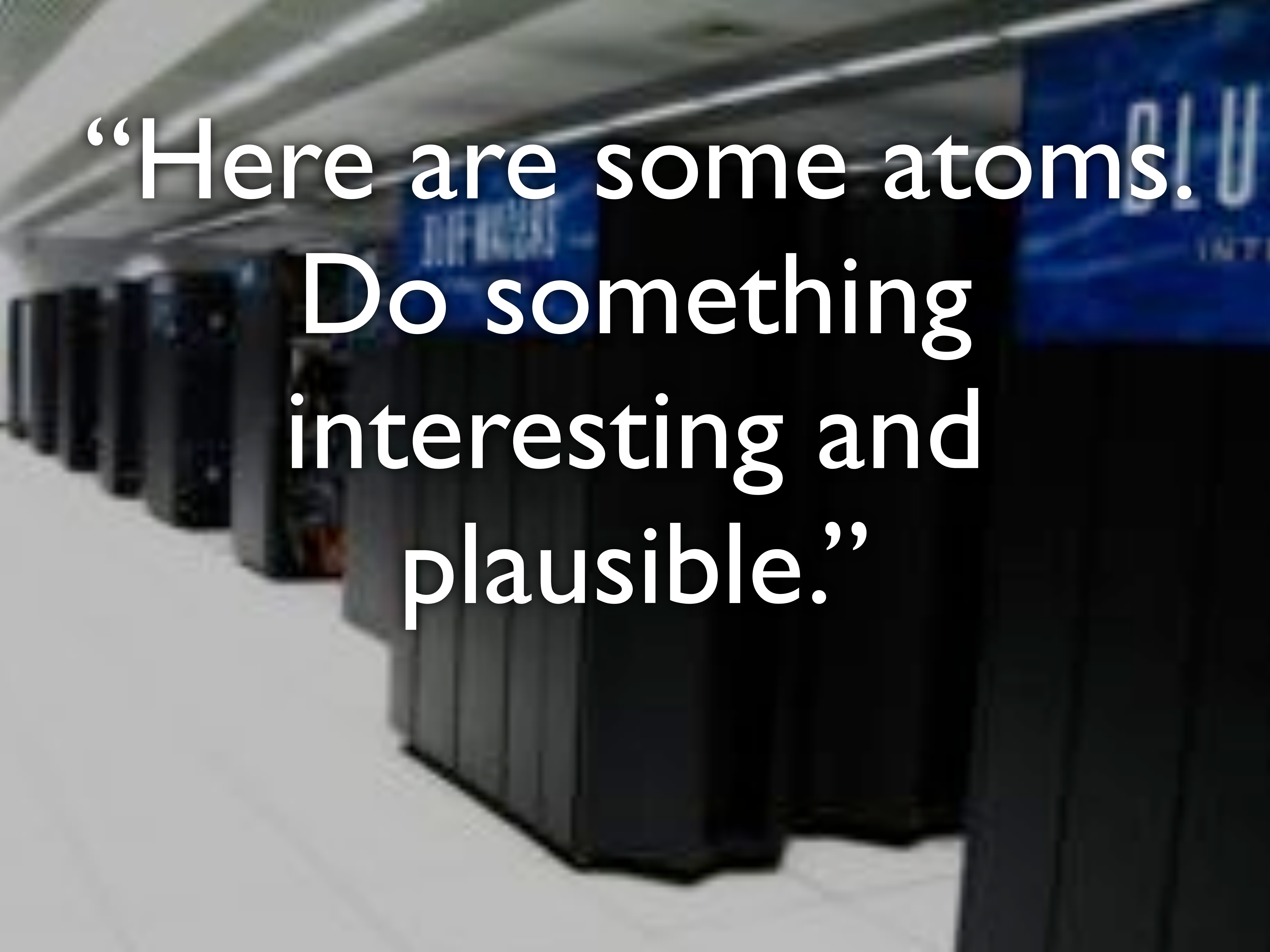


Information content of manifold of low-lying metastable states of a "Hubbard model" of chemistry

B-B bond strength



A-B, A-A bond strength


"Here are some atoms. Do something interesting and plausible."

Majid Nili
Jie Li
Sheng Zhang
Peter Schiffer
Nitin Samarth
Ruifang Wang
Xianglin Ke
Kito Holiday
David Stucke
Tyler Engstrom

ZhaoHui Huang

Cheng-Ing Chia

Youjian Tang

Feng Zhang

Paul Lammert

Postdoc

Faculty

Cristiano Nisoli

Ilya Grigorenko