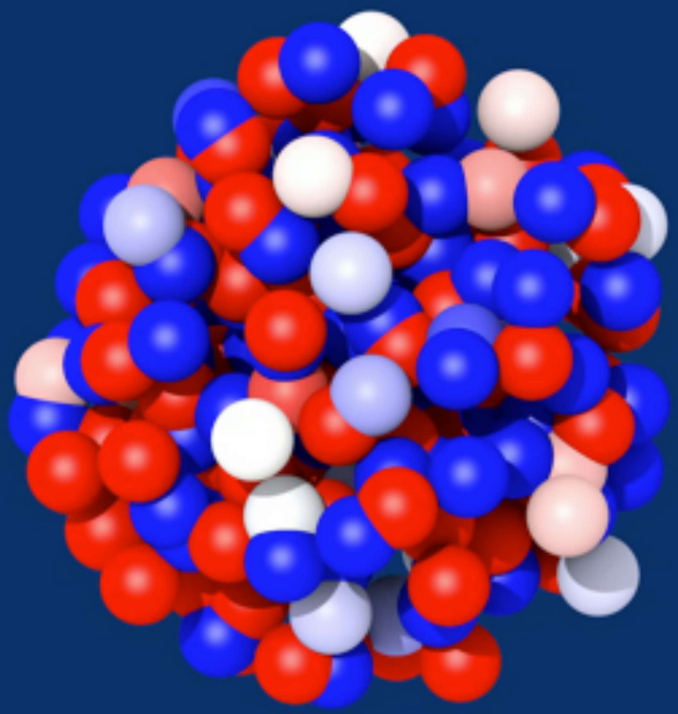
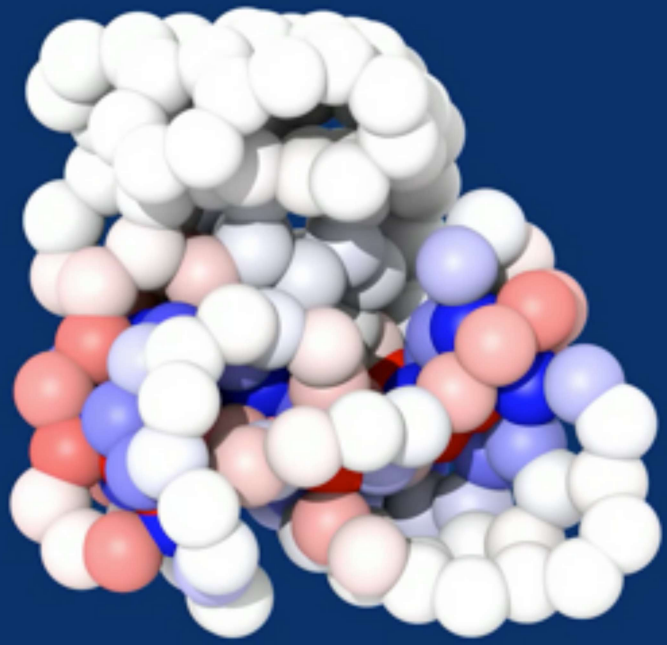
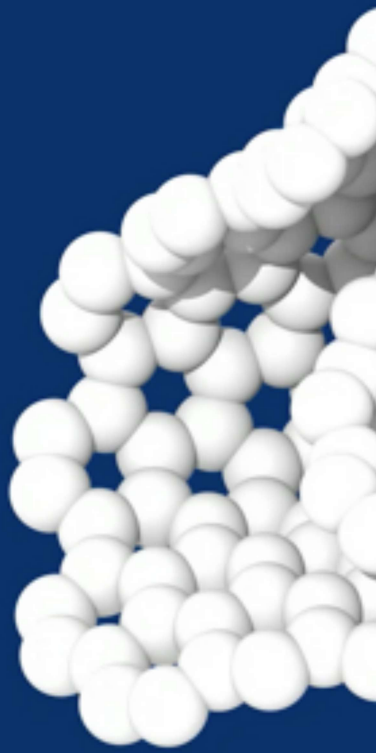
Stochastic samplin
dense matter



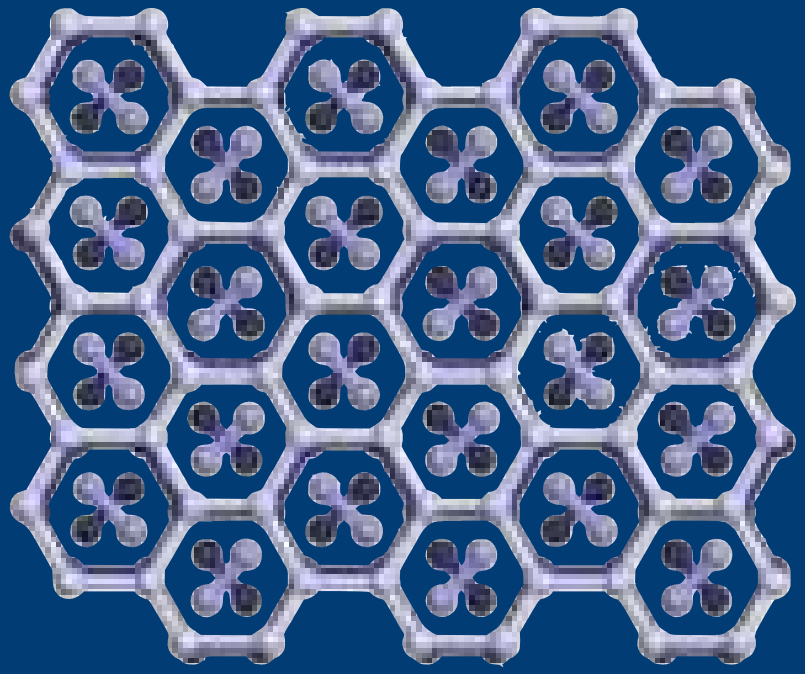




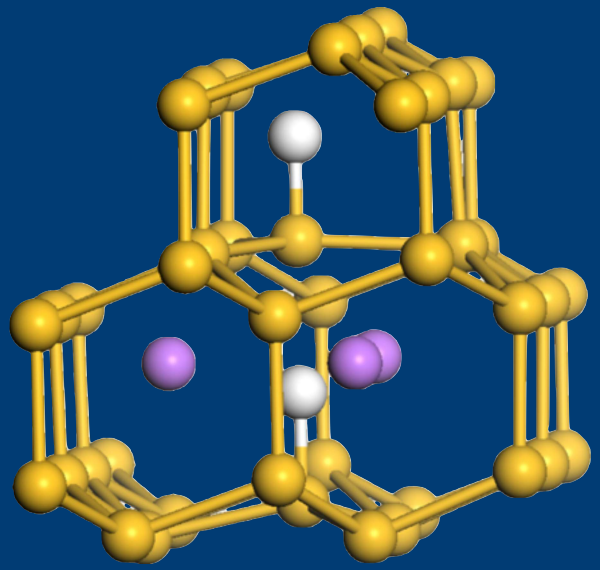
Chris J Pickard

Structure Predic

What structure will a collection
atoms adopt?



Crystal



Point Defect

Int

Energy

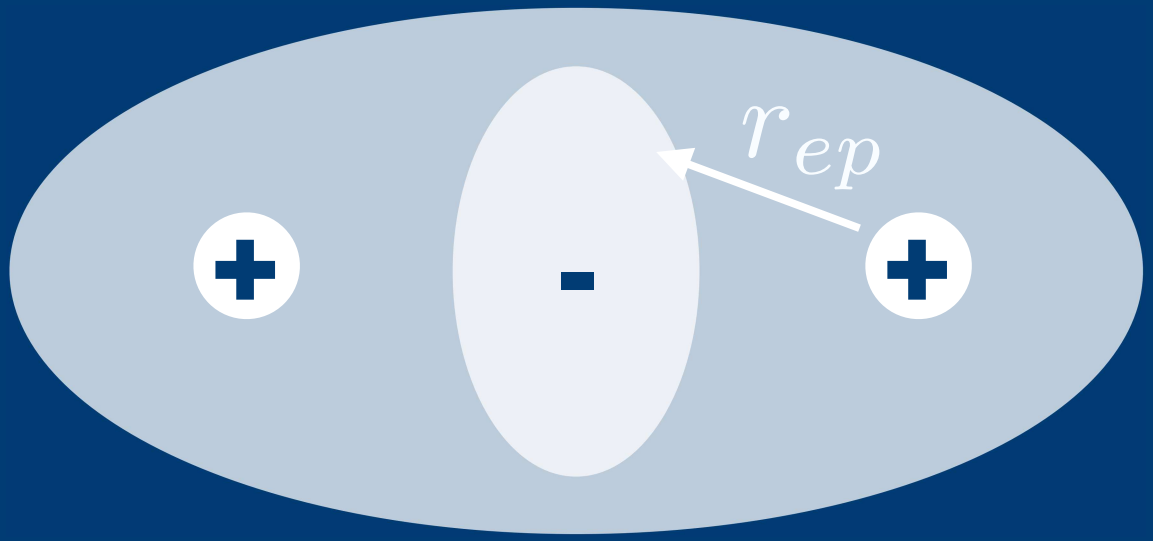
Interpolative

Empirical or data driven

Extrapolative and predic

First-principles or theory driven

Smooth interacti



$$E_{ep} = -$$

Coulo

$$H\Psi = -\frac{1}{}\nabla^2\Psi + V\Psi =$$

Smooth Landscap

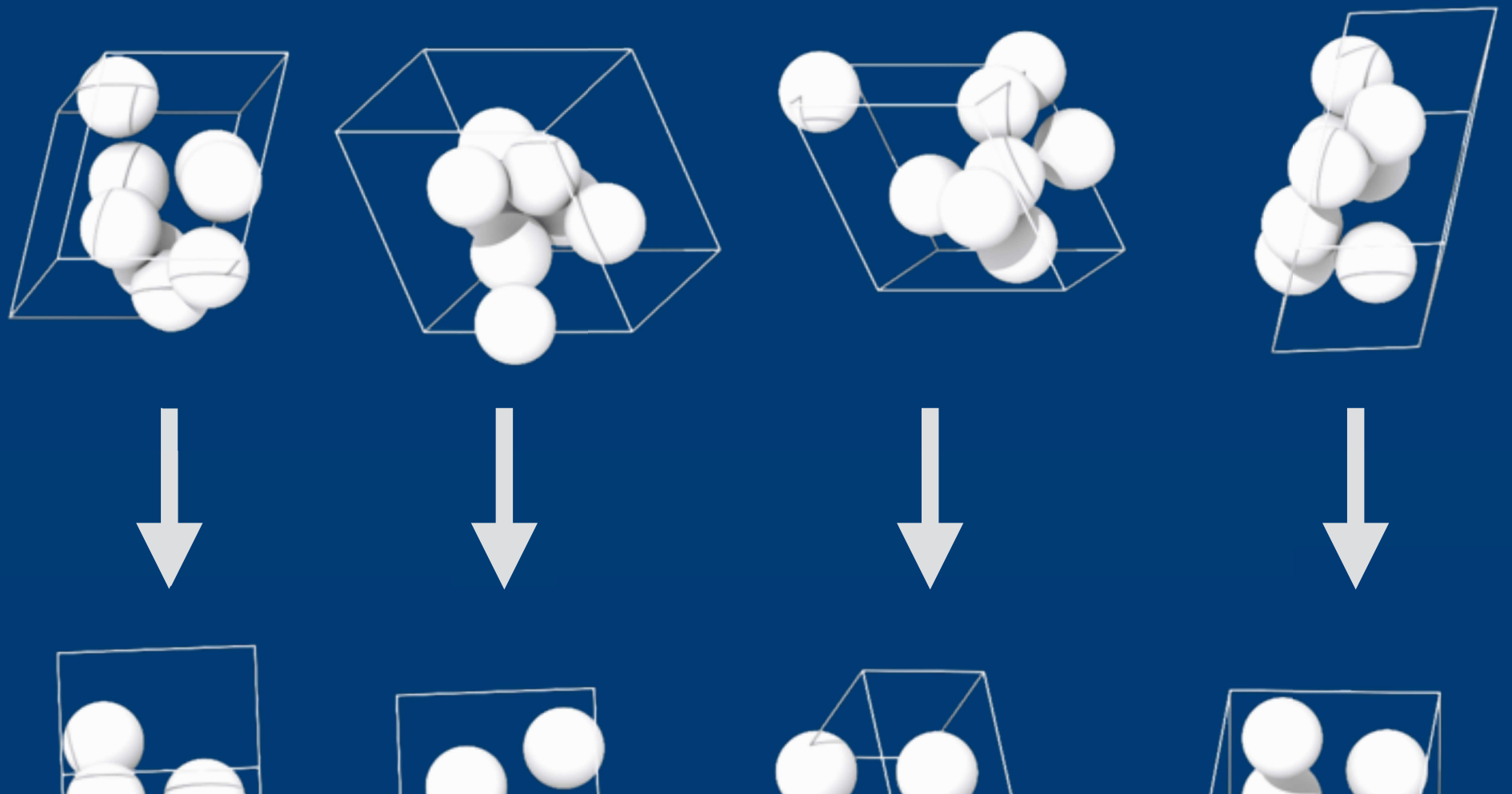
Smooth Landscap

Ab Initio Random
Structure Searchi

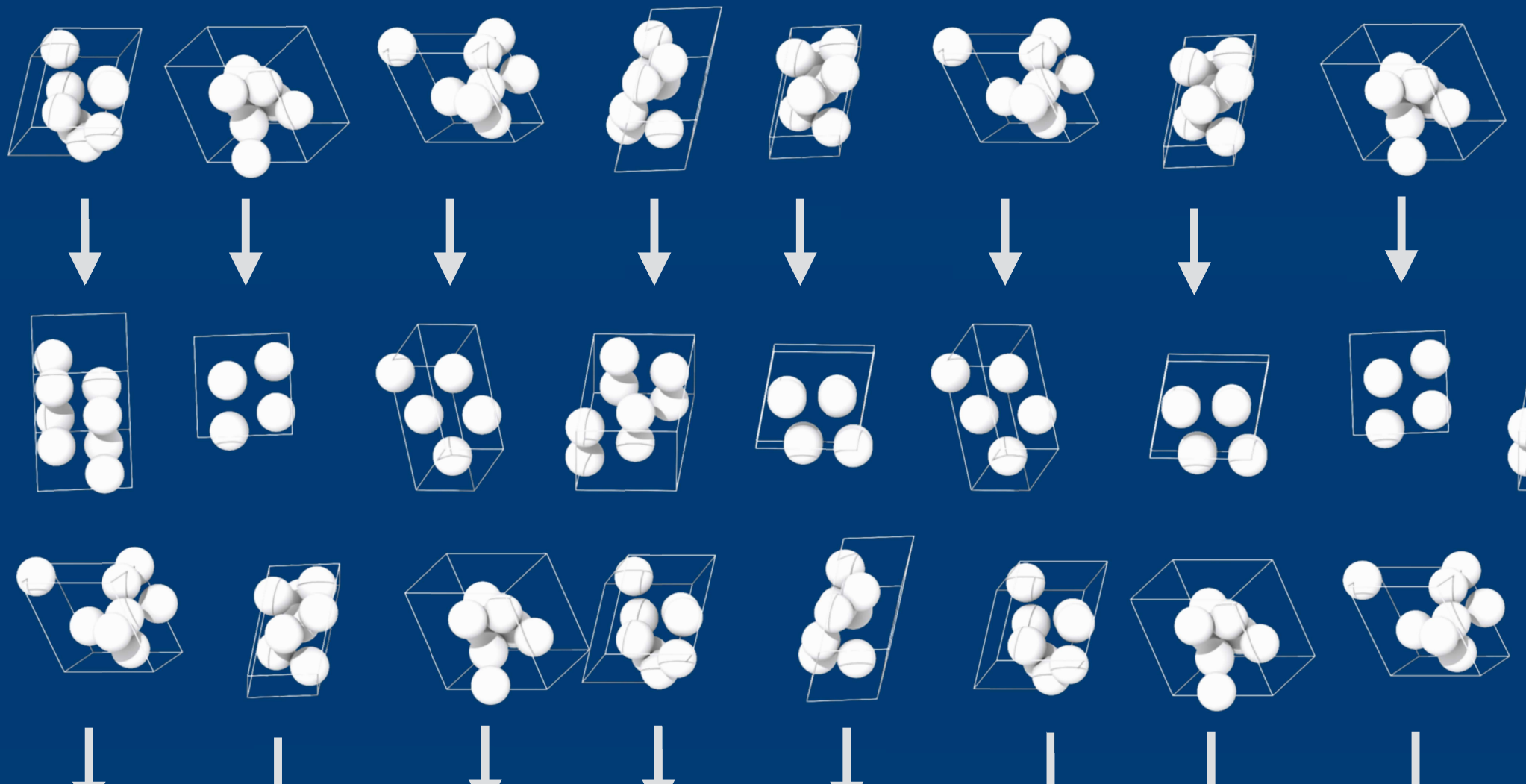
Pickard & Needs, *PRL* 2006 and *JPCM* 20

Local
optimisation

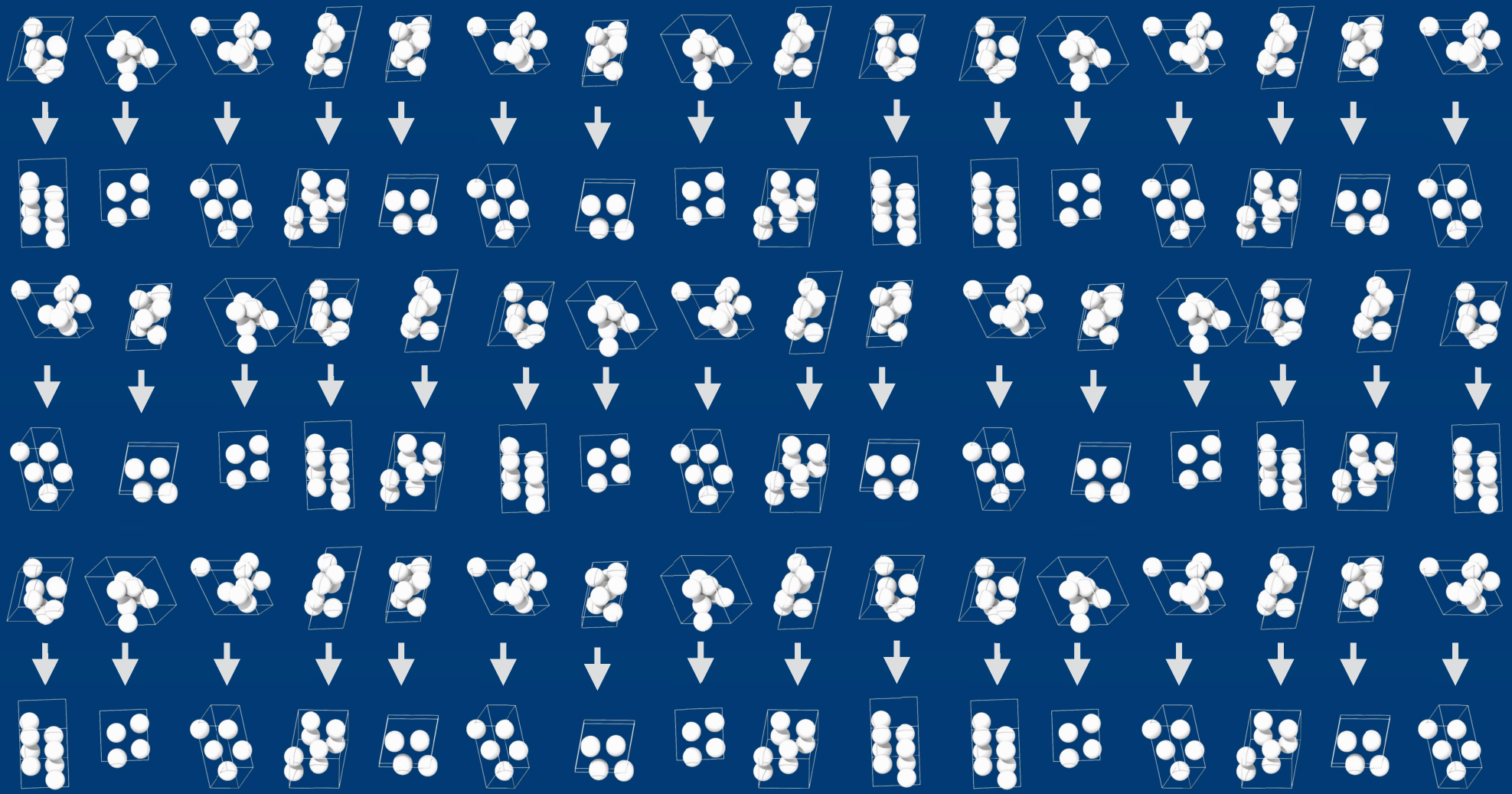
Ab Initio Random Structure Searchi



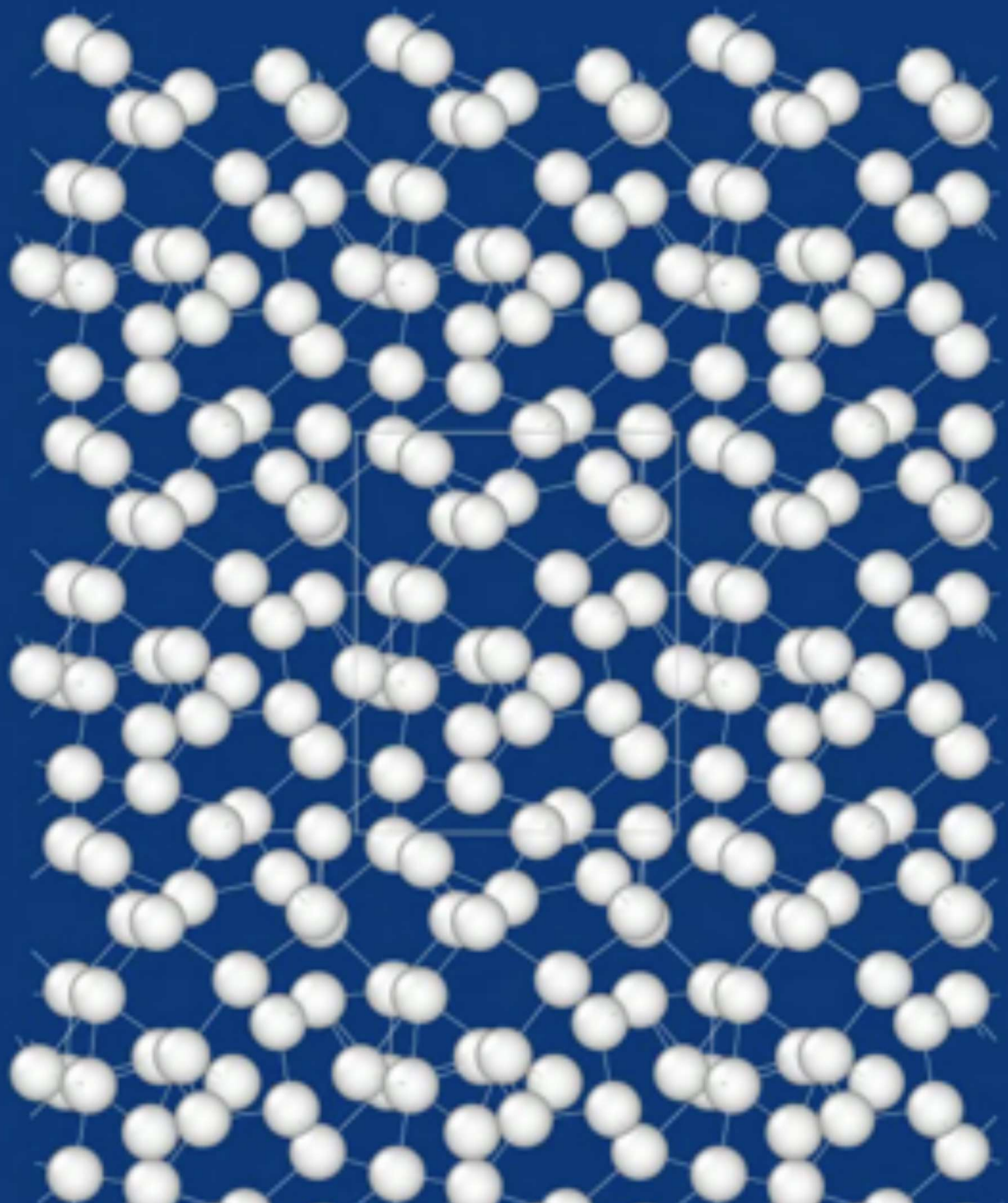
Ab Initio Random Structure Searchi

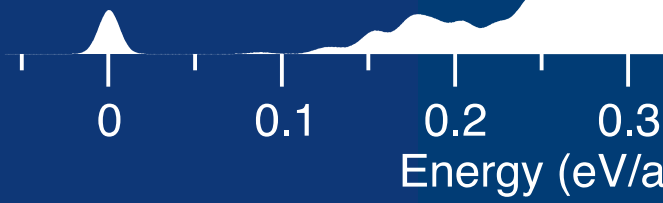


Ab Initio Random Structure Searchi

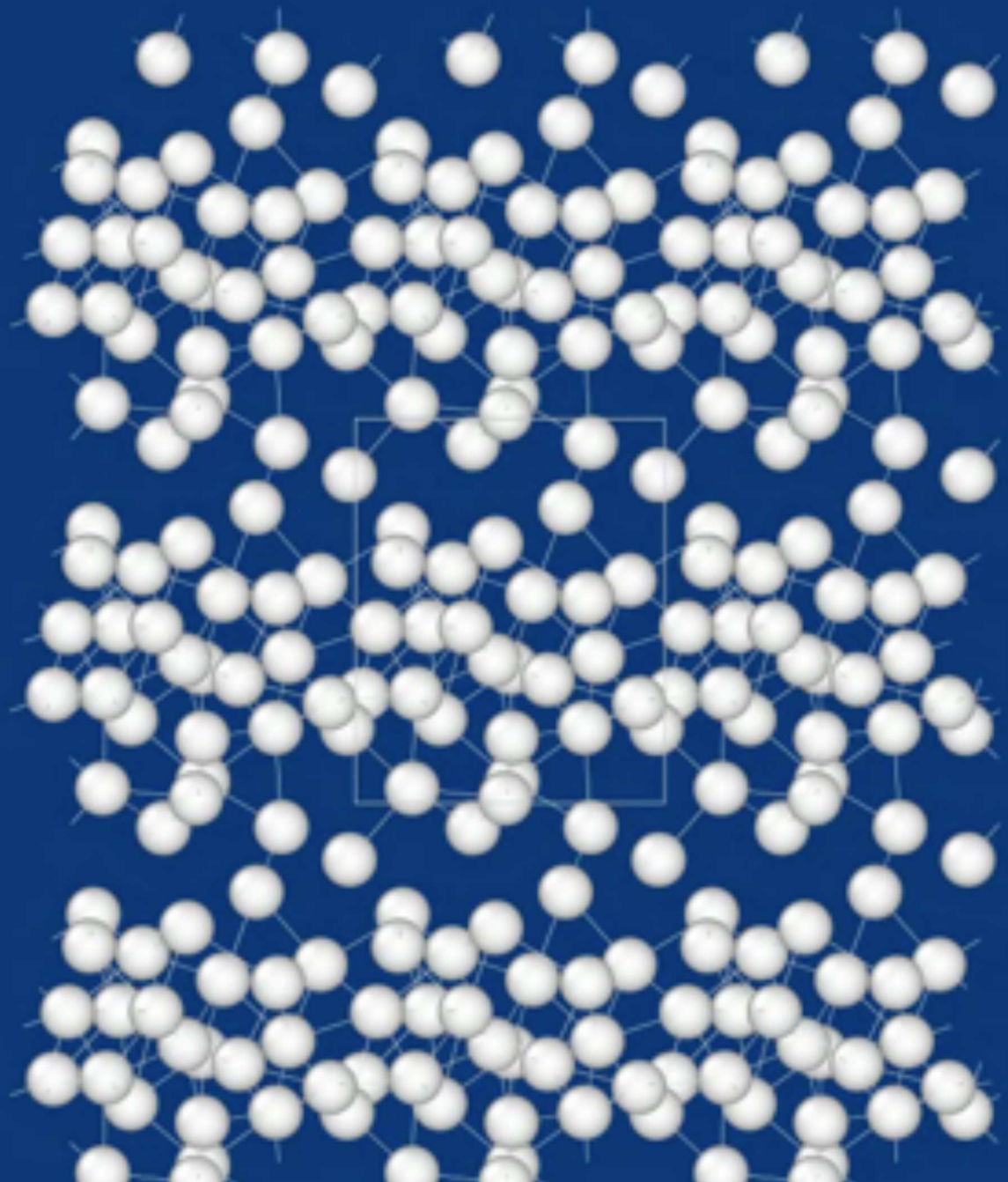


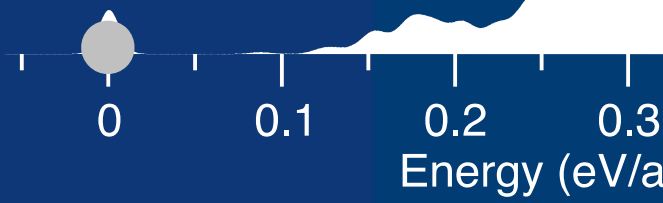
Gamma Boron





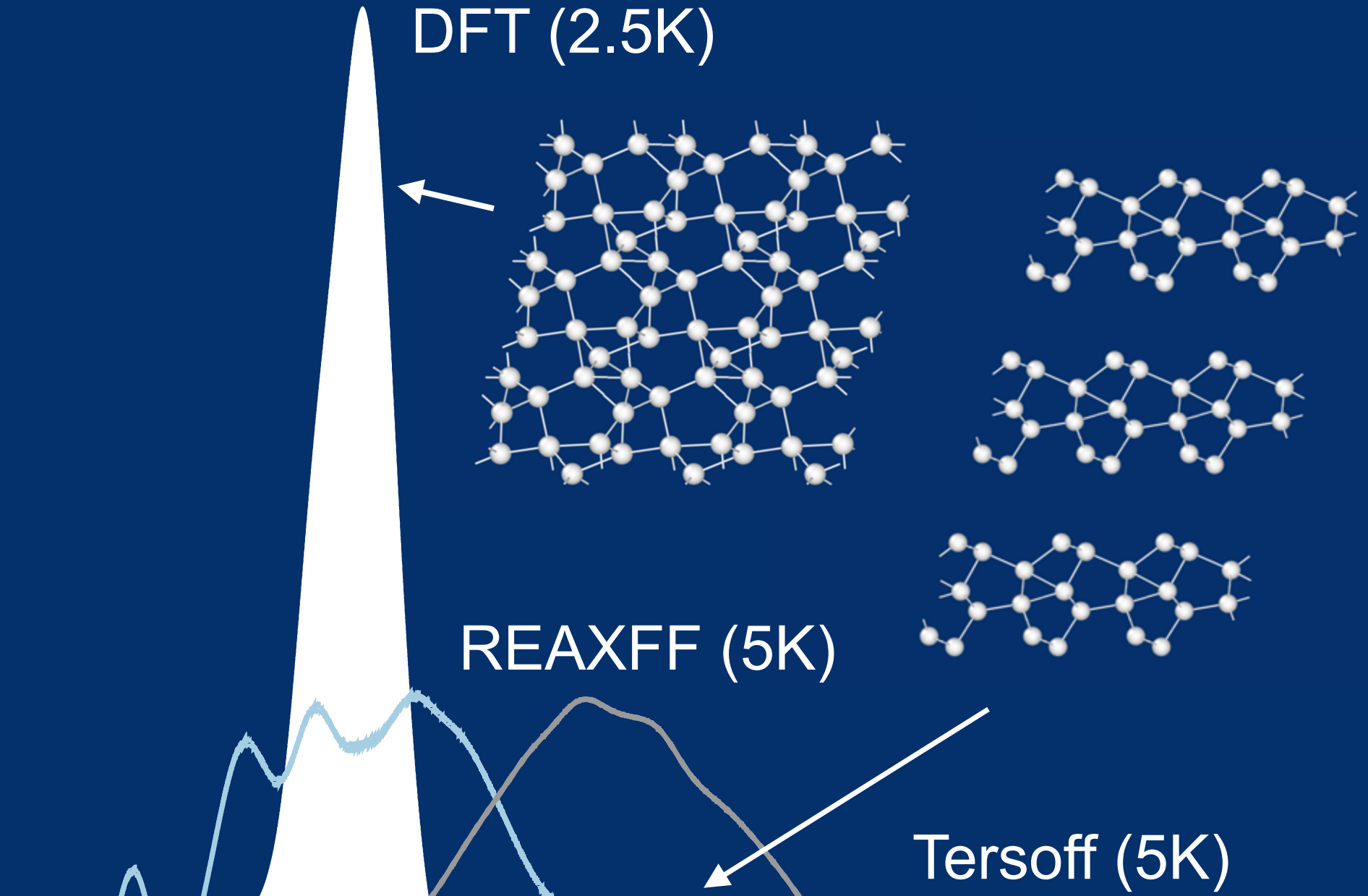
Gamma Boron



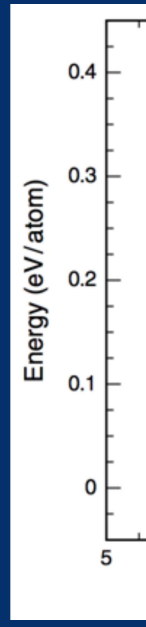


Data Driven or First Princ

Eight atoms of Silicon



Data
of
Ener



De
Csa

Random Structure Searchin

Uniform distribution
(*exploration*, no *exploitation*)

Intrinsically parallel

Uncorrelated

Clear when (not) to stop

Being Sensibl

When you don't know anything

rough volume, avoid overlap - Poisson Disk

Impose chemical ideas

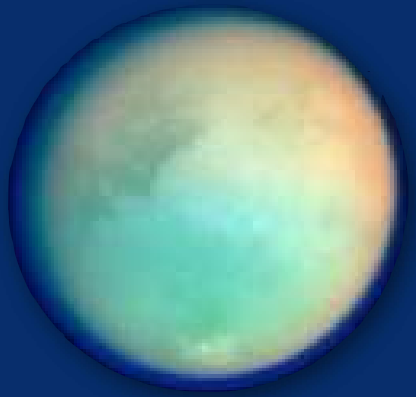
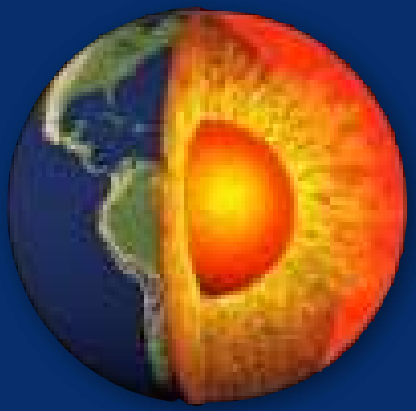
molecules, fragments, distances, connectivity

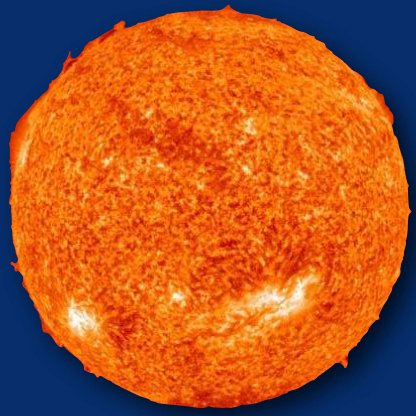
Impose symmetry

space, wallpaper, point group

Condensed matte

$$H = U + pV$$





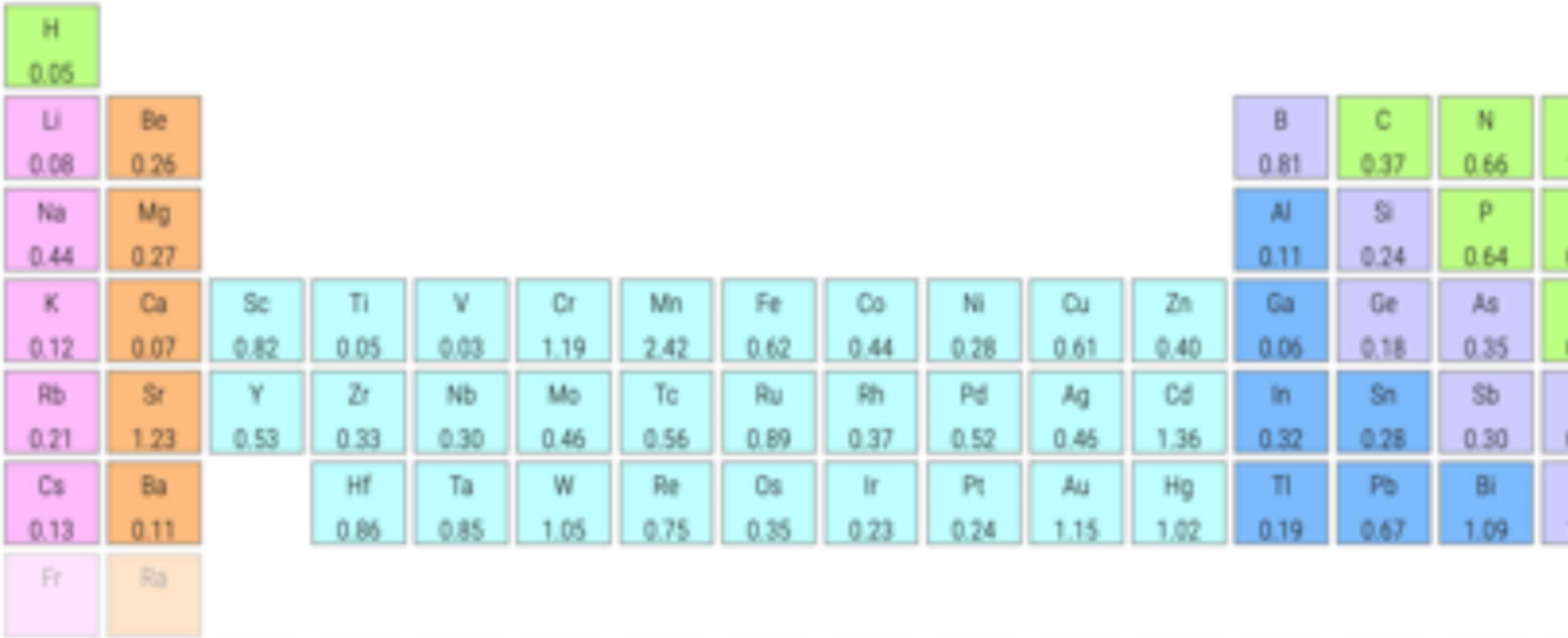
Potentials

Reference point: WIEN2k13.1 with basis LAPW/APW+lo and potential all-electron

Code: CASTEP9.0 with basis plane waves and potential OTFG CASTEP 9.0

Maximum at Mn. Minimum at V

All values are in meV.



Potentials

Reference point: WIEN2k13.1 with basis LAPW/APW+lo and potential all-electron

Code: CASTEP9.0 with basis plane waves and potential OTFG CASTEP 9.0

Maximum at Mn. Minimum at V

All values are in m

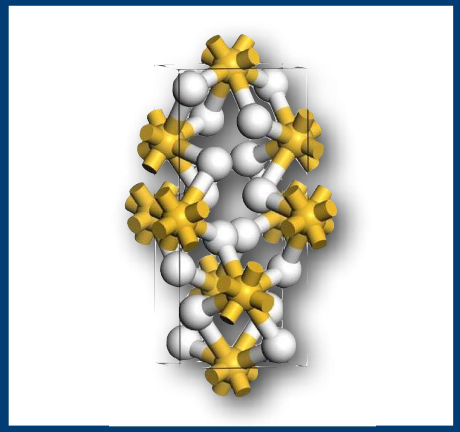
H 0.05																	
Li 0.08	Be 0.26																
Na 0.44	Mg 0.27																
K 0.12	Ca 0.07																
Rb 0.21	Sr 1.23																
Cs 0.13	Ba 0.11																
Fr	Ra																

```
#VARVOL=2
#SPECIES=C
#NATOM=4
#MINSEP=0.5

KPOINTS_MP_SPACING 0.05

%BLOCK SPECIES_POT
C 2|0.75|30|34|39|10U:20:21(qc=1
%ENDBLOCK SPECIES_POT
```

Discoveries in dense matter

Superconducting hydrides?

Physical Review Letters, 2006



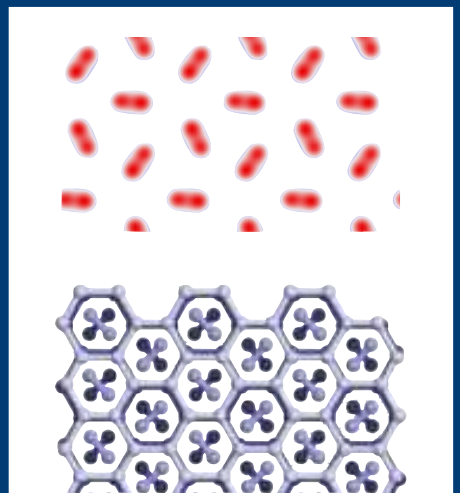
The end of wate

Physical Review Letter 2013

+ Martinez-Canales

Hydrogen is polar and "graphene"

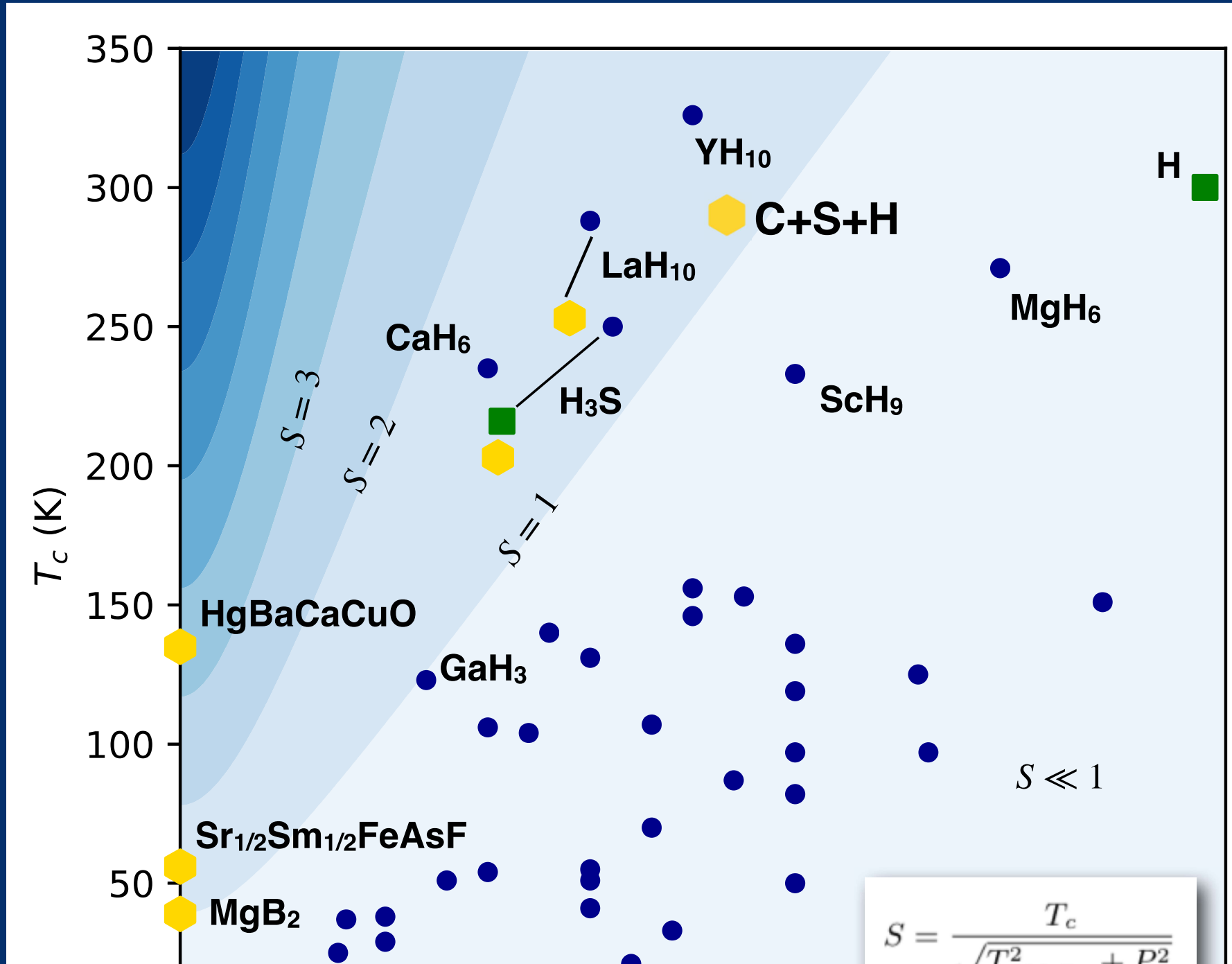
Nature Physics,



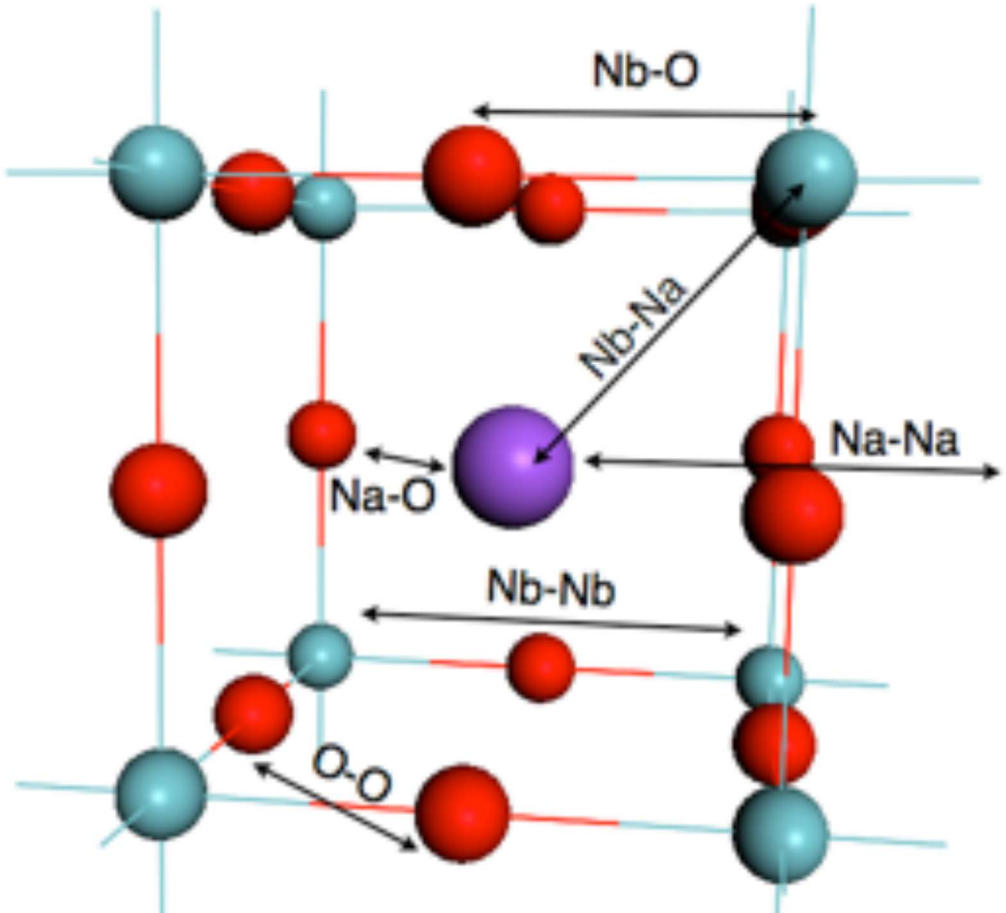
Aluminium is complicated

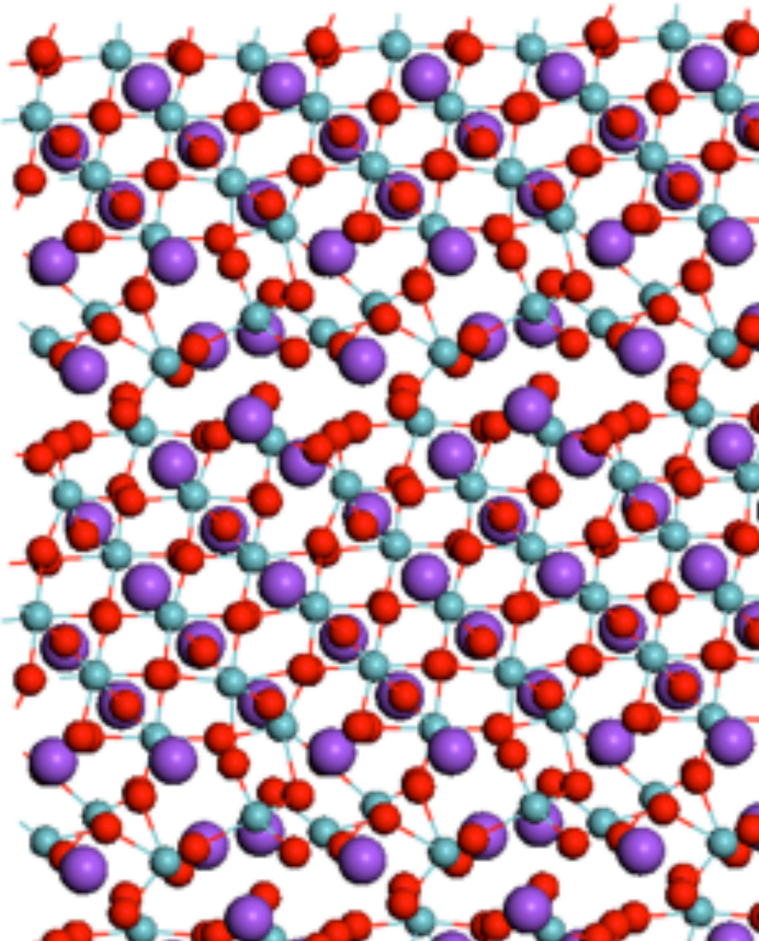
Nature Materials,

Superconducting Hydri



Increasingly sensi
structures





New directions

Allow the particles making up a struc
explore a higher dimensional ***physica***

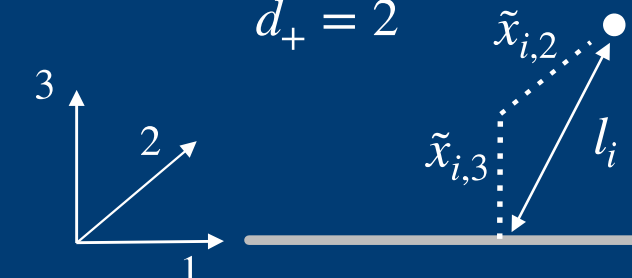
$$d = d_0 + d_+$$

Hyperspace — Normal space — Extra dimensions

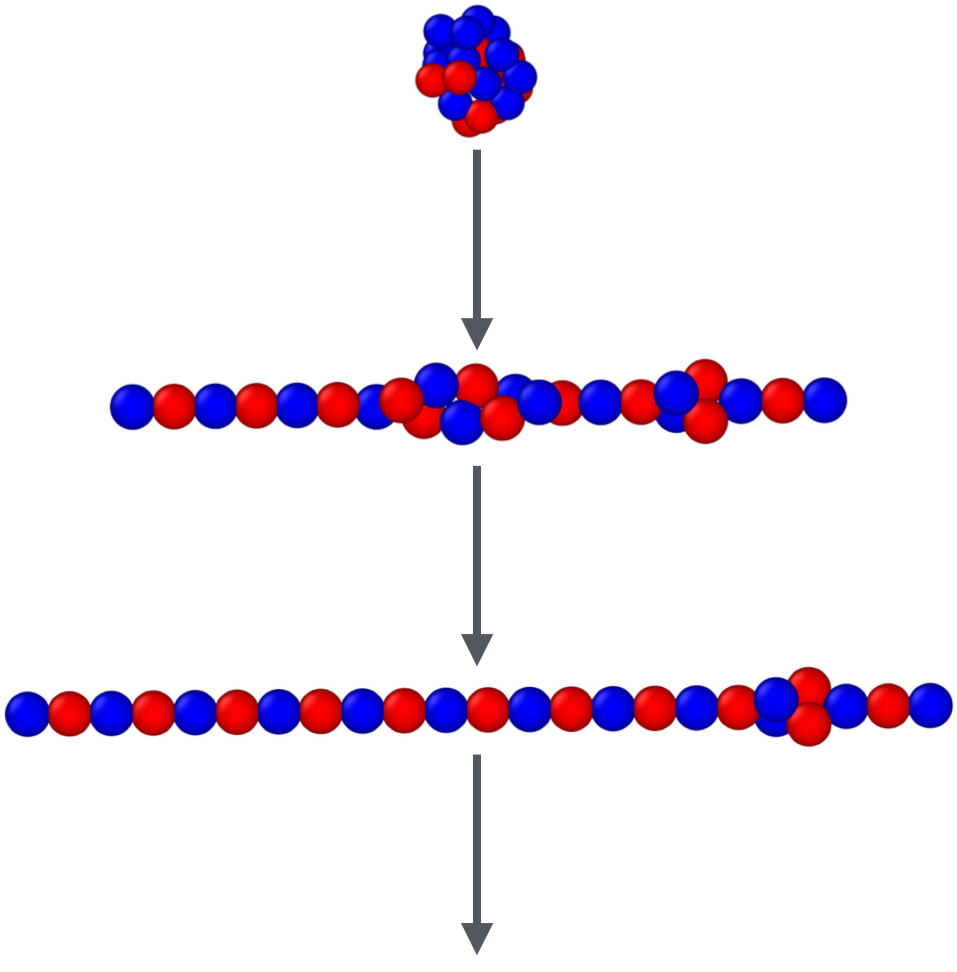
$$\bar{E}(\{\tilde{\mathbf{x}}_i\}) = \tilde{E}(\{\tilde{\mathbf{x}}_i\}) + \frac{1}{2}\mu \sum_i l_i^2$$

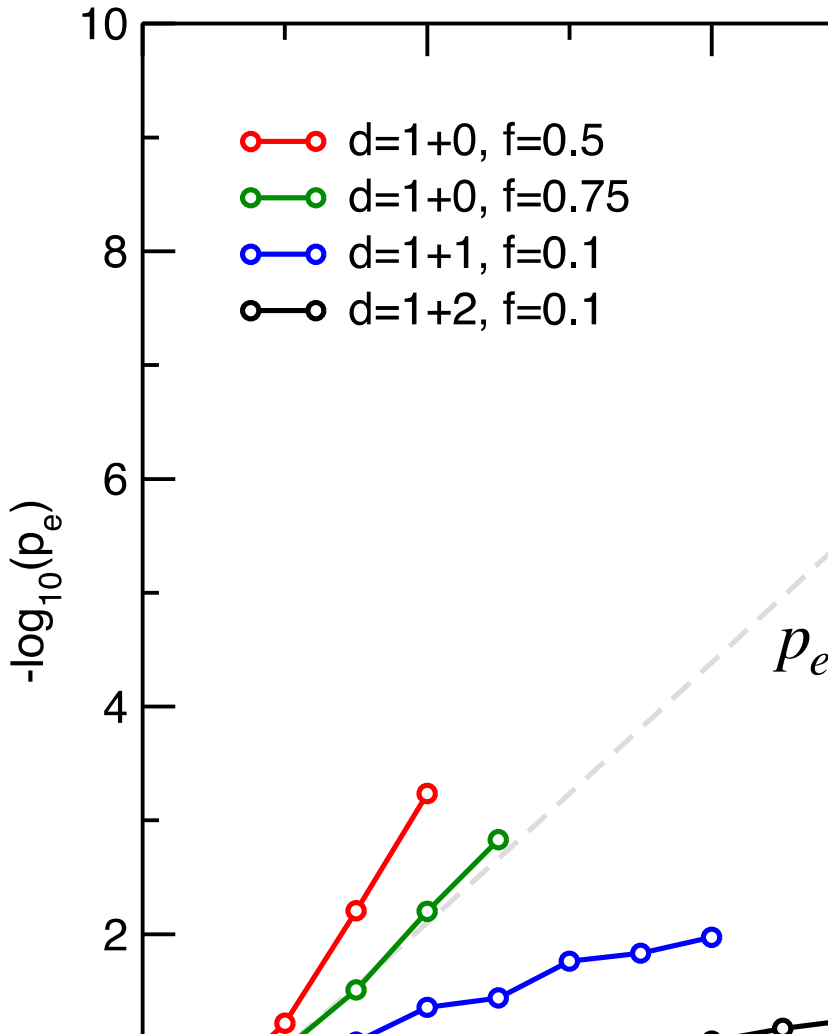
Energy extended to

Increasing

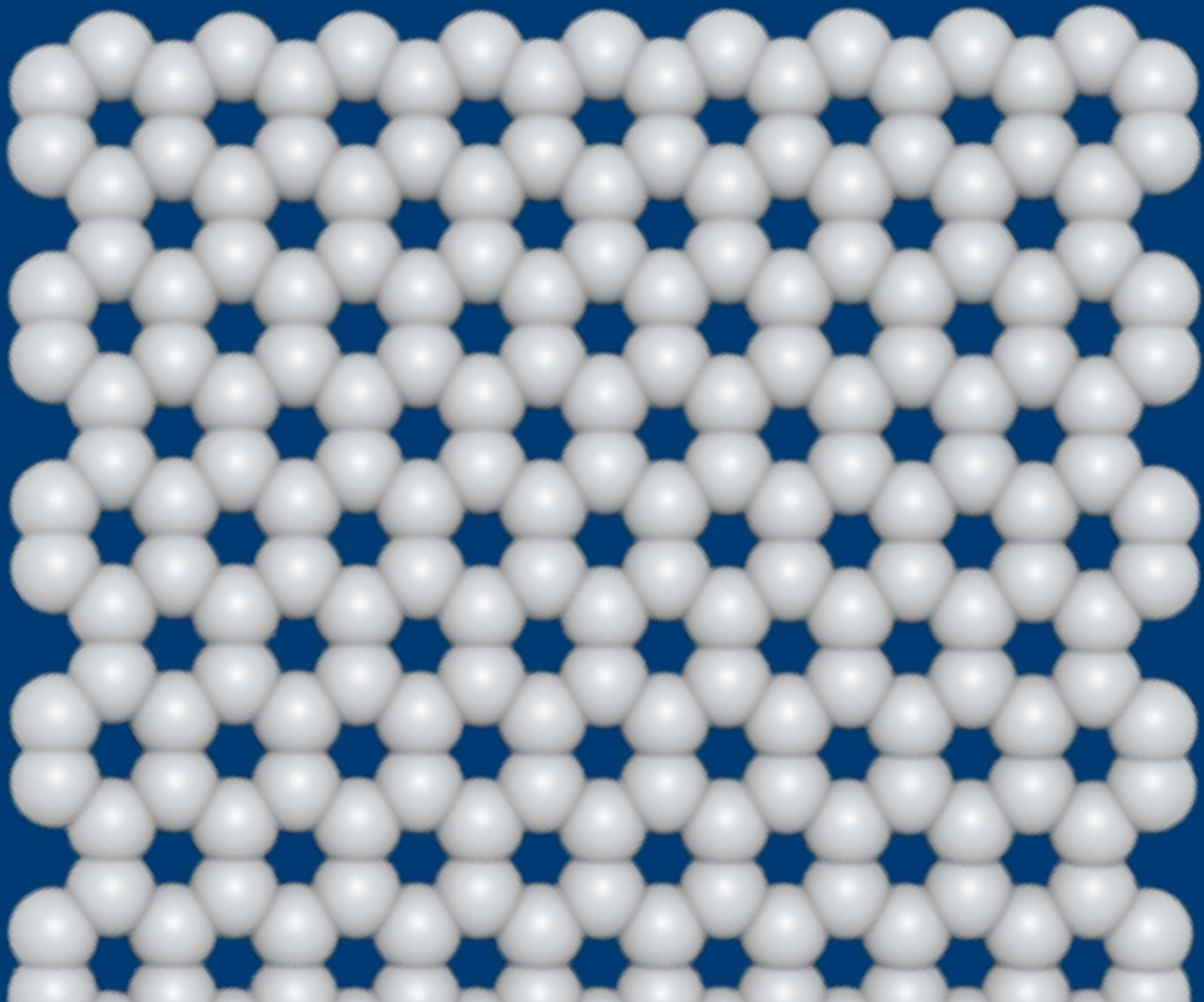


Binary chain

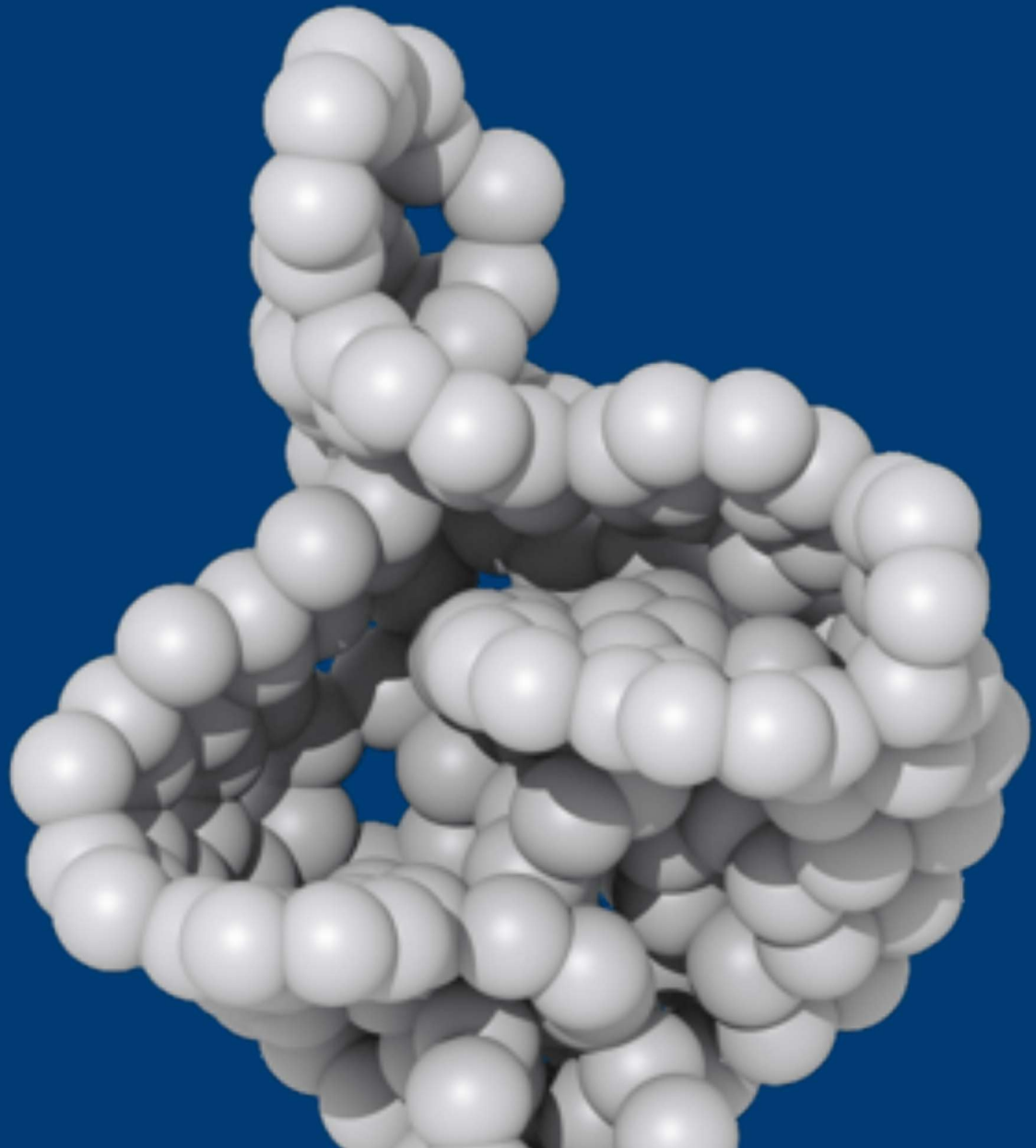


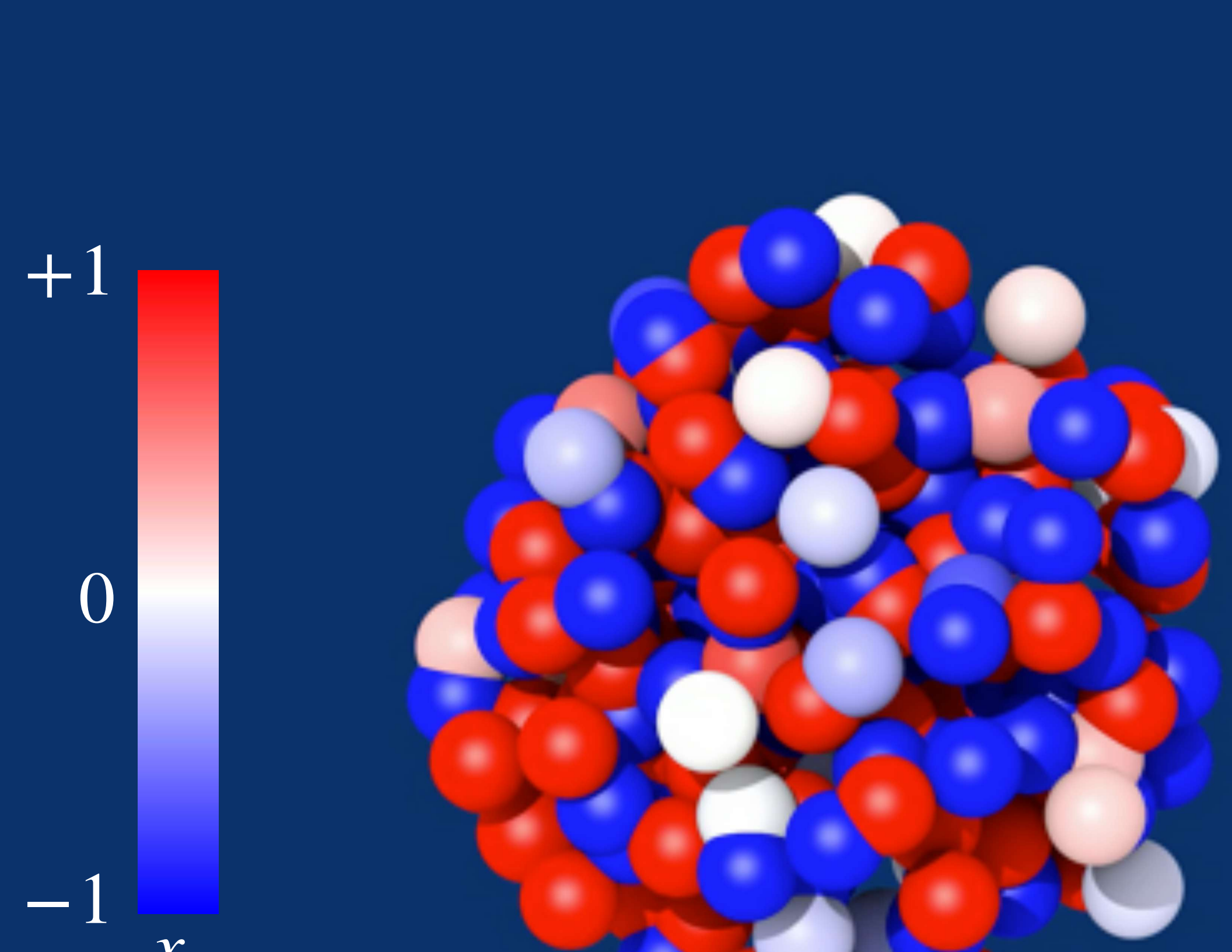


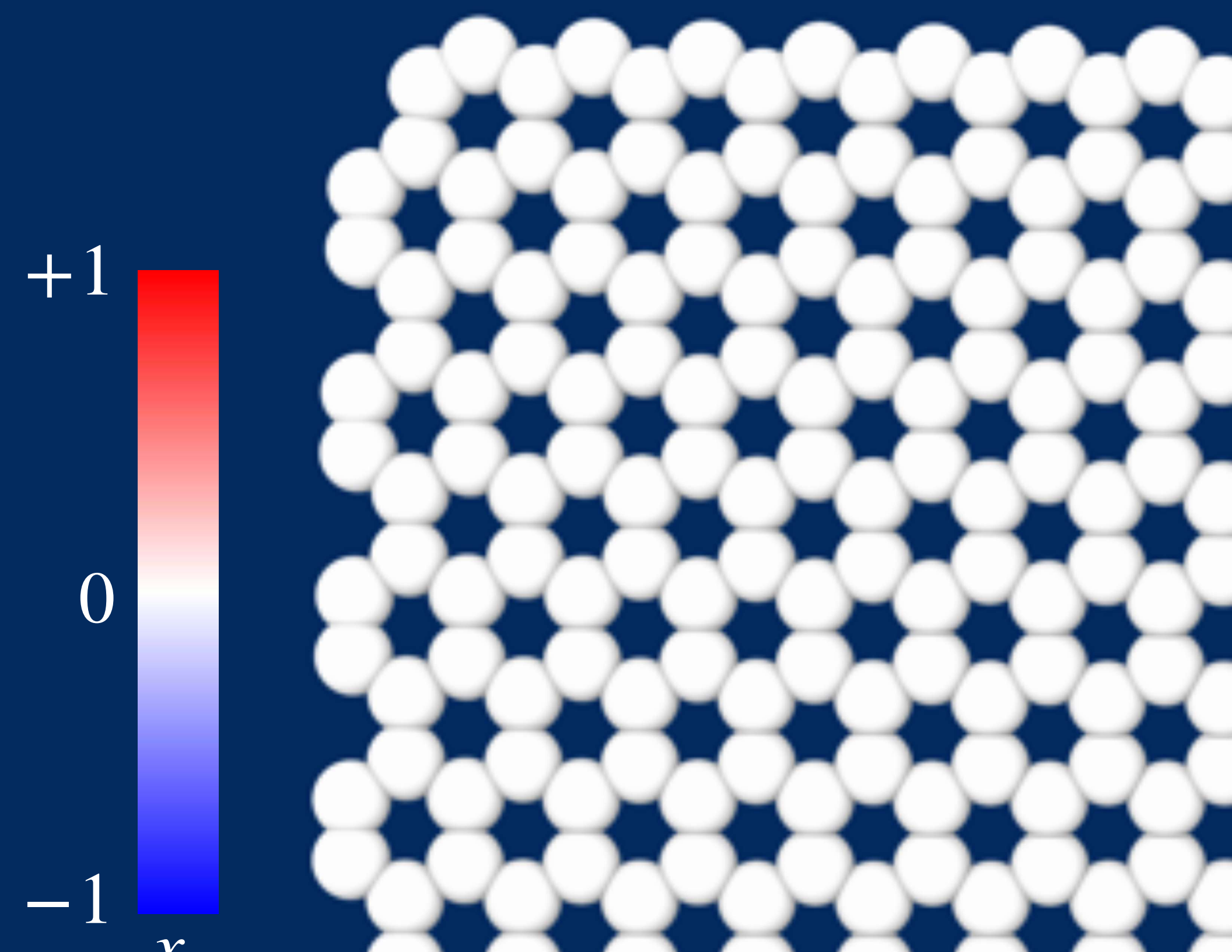
Covalent bonds



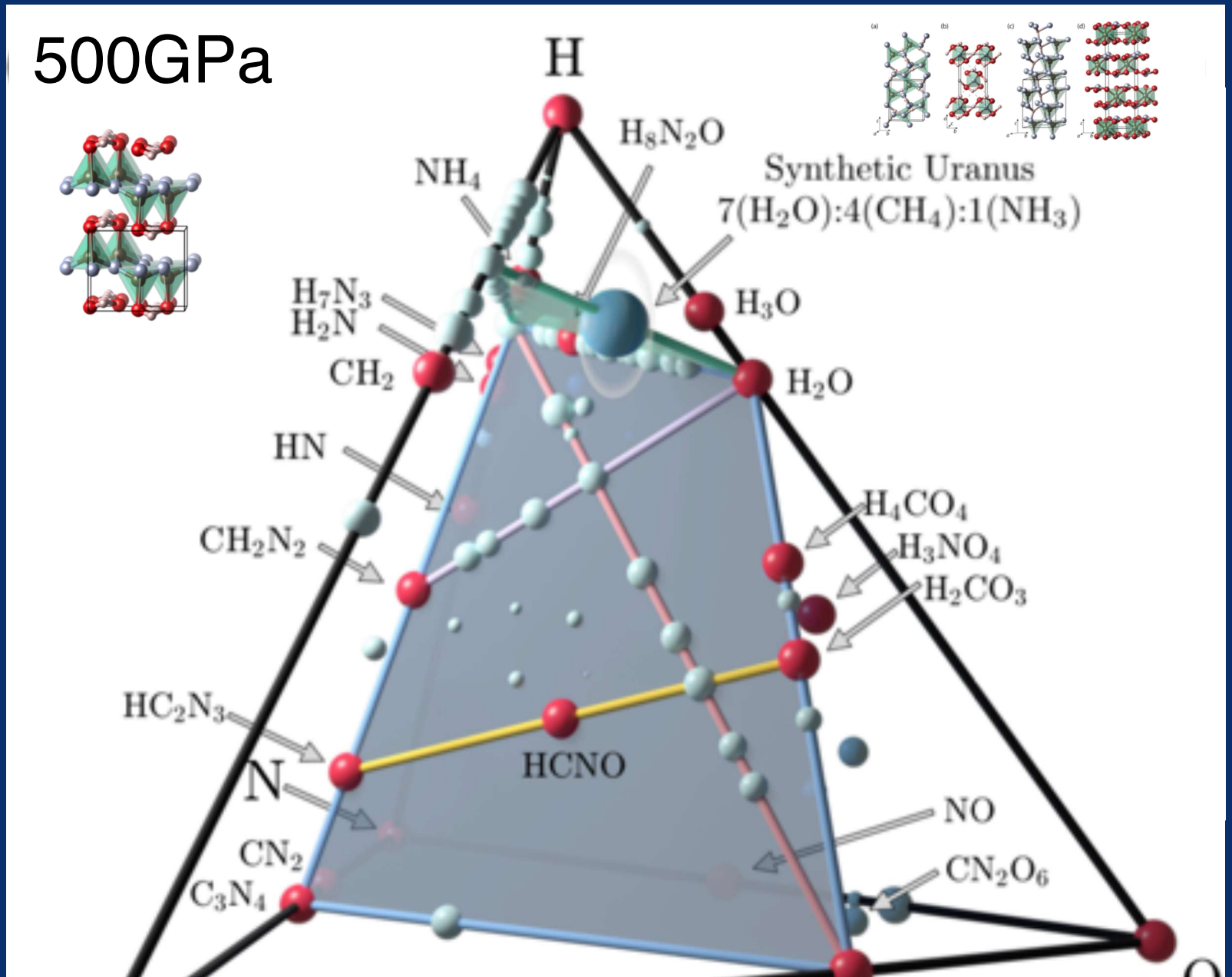
Covalent bonds




+1
0
−1
x


+1
0
−1
x

H-C-N-O



1. The C
rules - di
HC

2. S
comp
relatively
p

3. Realist
don't
decom

Conclusion

Stochastic search and first princip
approaches can ***discover***

They can be used as ***virtual***
experiments in dense matter

CASTEP now available cost free f
academic research globally

AIRSS package available from: