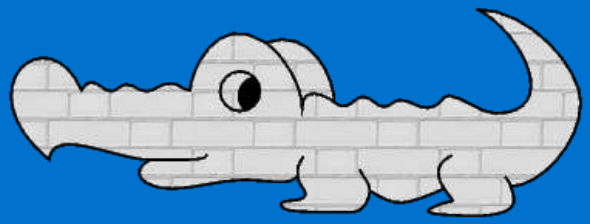
UNIVERSITY OF CAMBRIDGE

Dragons' Den



Gareth Conduit
Matthew Evans, Nicolo Forcellini, Will Grant, Mark Johnson, Alexander Leonard, Yang Liu, Ezequiel Rodriguez Chiacchio, Matthew Smith, Stephen Spurrier, Philipp Verpoort, Lupeng Yang

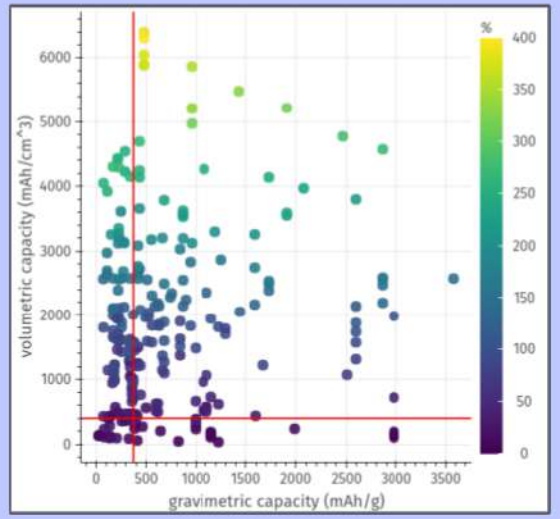
Theory of Condensed Matter

Crystal structure prediction for conversion electrodes

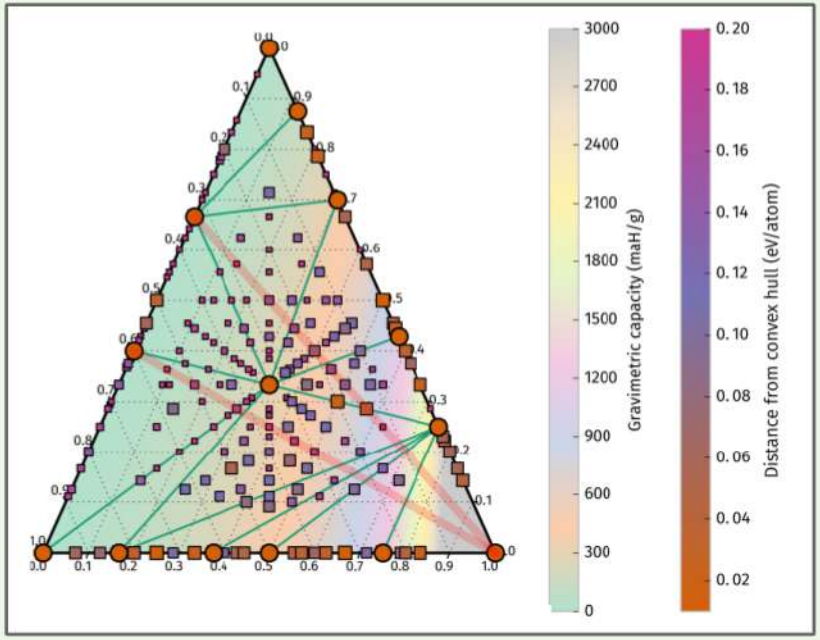
$$X_xY_y \longrightarrow nAX_x + n'AY_y$$

maximise gravimetric capacity
with
manageable volume expansion

MATADOR + mongoDB



AIRSS + CASTEP



High-throughput prediction and refinement:

- electrochemical performance
- spectroscopic properties

Matthew Evans

EPSRC Centre for Doctoral Training | Computational Methods for Materials Science

Supervisor: Andrew Morris

Radiation Damage

A Floquet-Bloch approach

- Damage caused by radiation is a major issue for structural materials in fission and fusion reactors and in many other applications.
- Theoretical models are necessary to understand what happens during these processes.
- An explicit treatment of the electrons is important, especially for fast projectiles (E/W $\gtrsim$ 10MeV).
- A Floquet-Bloch theory, which combines discrete time and spatial translation symmetry, could provide a more general model to study the (non-adiabatic) electronic response.

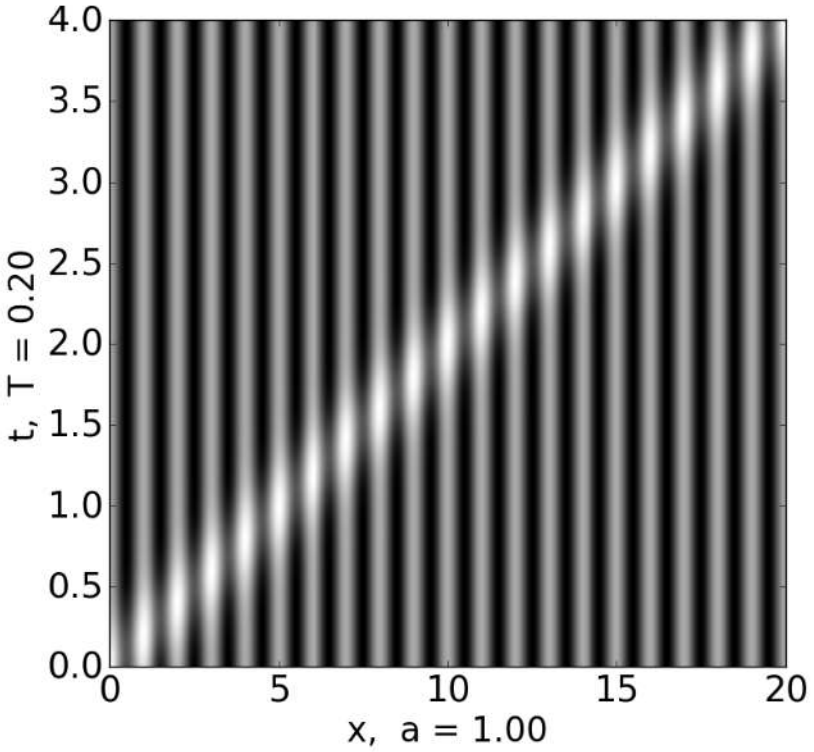
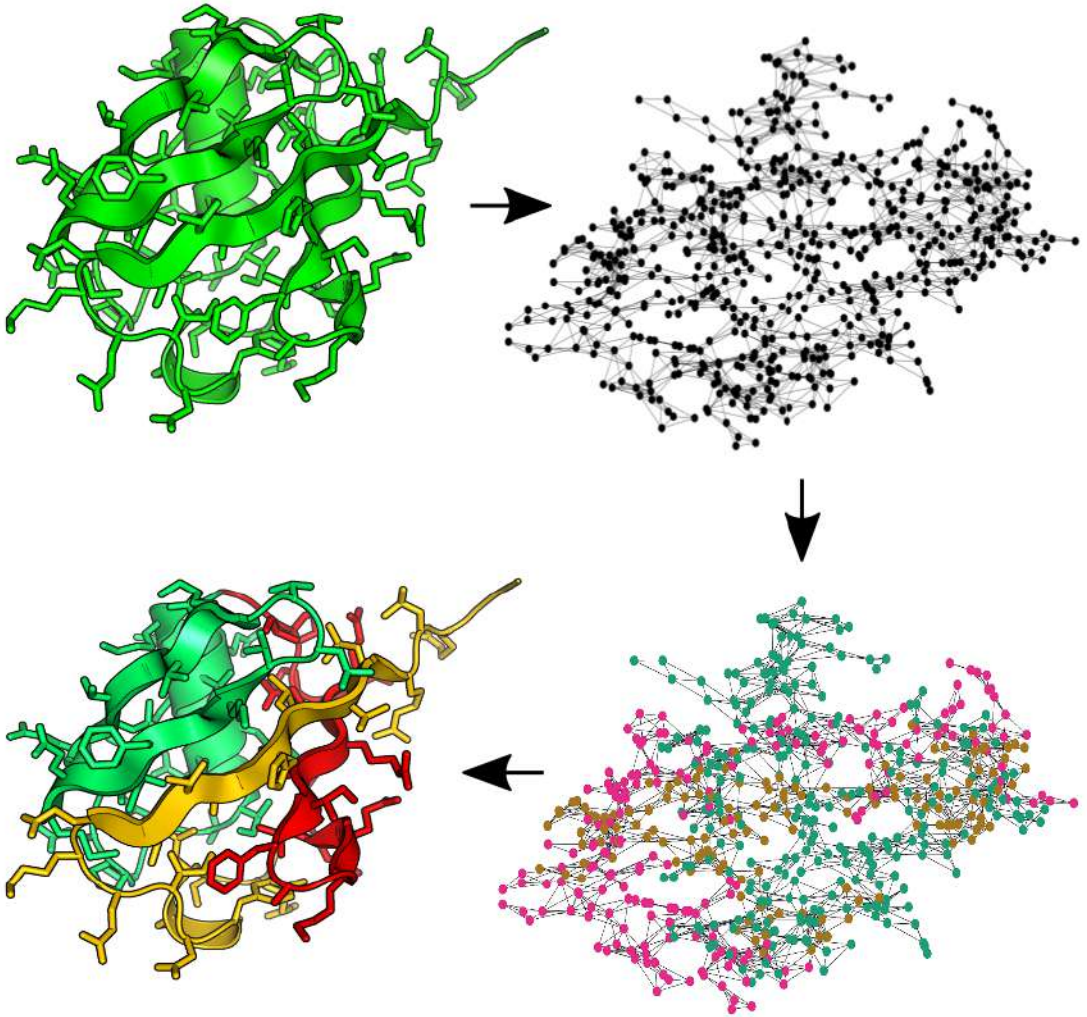
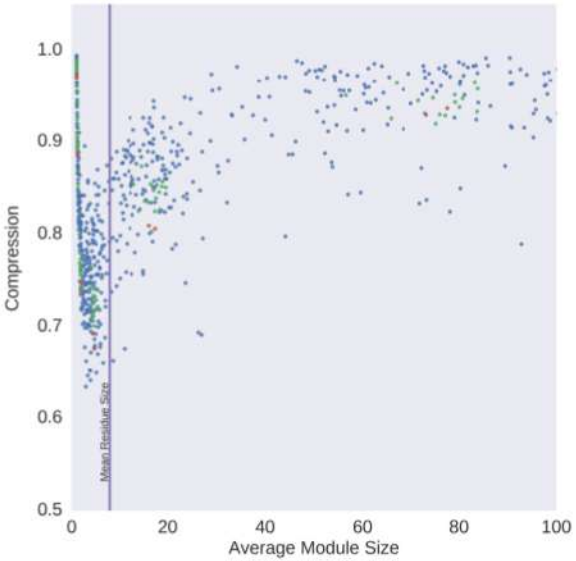
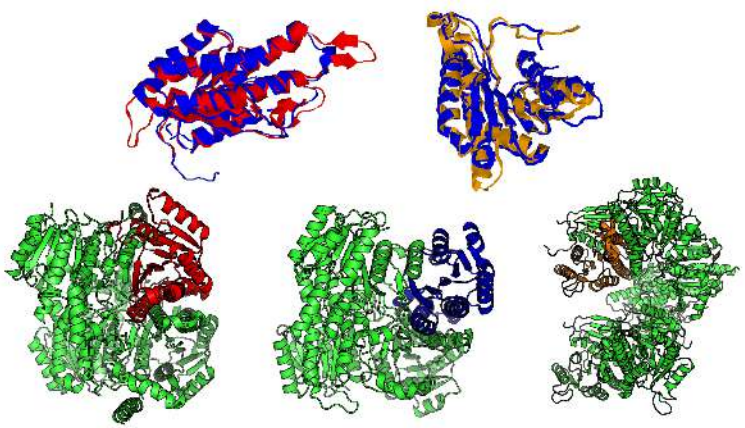


Figure: Simplified graphic representation of a 1-dim lattice with lattice spacing a, with a projectile crossing it with velocity $v = a/T$. Arbitrary units.

Network Analysis of Protein Structure







William Grant / Sebastian Ahnert & Chris Pickard

EPSRC

Born-Oppenheimer approximation:

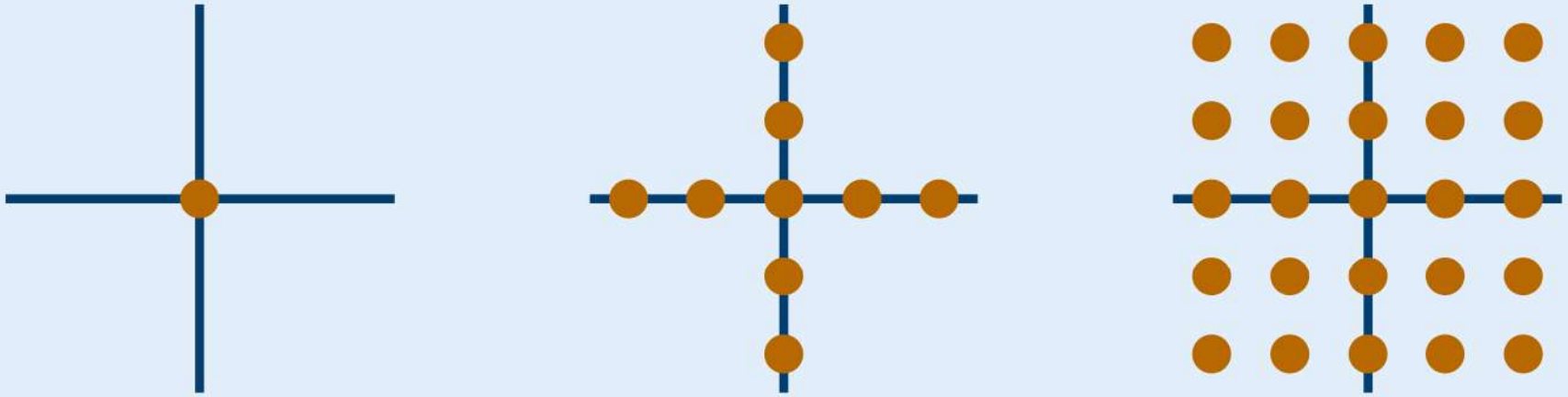
$$\mathcal{H}_{\mathrm{BO}} = -\frac{1}{2}\sum_i \frac{\partial^2}{\partial \mathbf{q}_i^2} + V(\{\mathbf{q}_i\})$$

Vibrational self-consistent field:

$$|\Psi_k\rangle = \prod_j a^\dagger(\mathbf{q}_i)\,|0_k\rangle \qquad ; \qquad \widetilde{V_k^j} = \langle\Psi_k|\, a(\mathbf{q}_i)\, V\, a(\mathbf{q}_i)\,|\Psi_k\rangle$$

Multi-mode expansion:

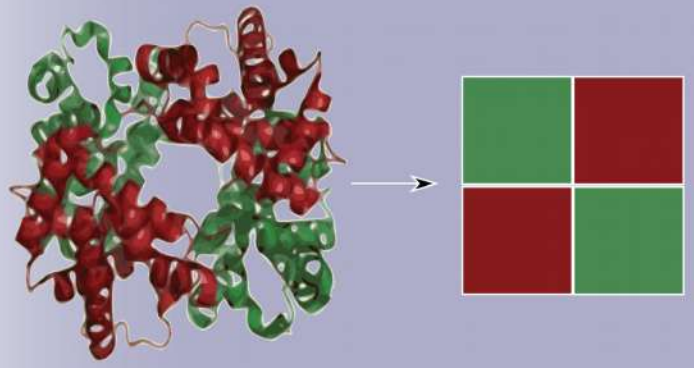
$$V = \quad V^{(0)} \quad + \quad \sum_i V^{(1)}(\mathbf{q}_i) \quad + \quad \sum_{i,j} V^{(2)}(\mathbf{q}_i, \mathbf{q}_j) + \cdots$$



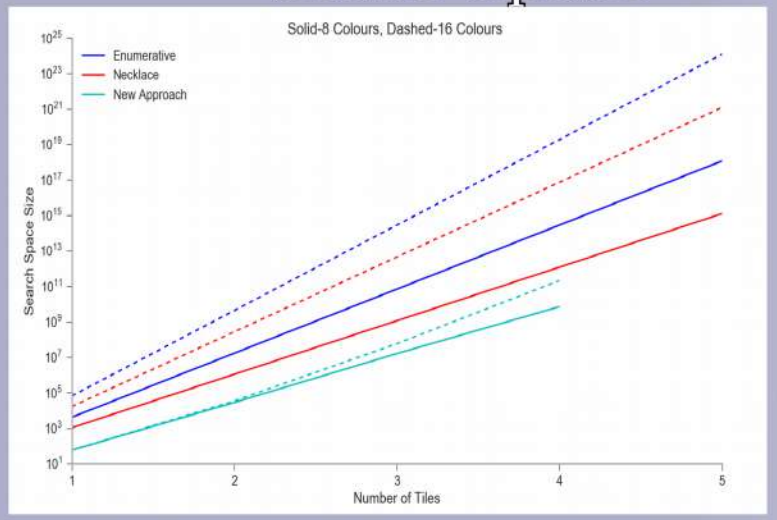
Proteins and Polyominoes

Looking at Genomic Evolution

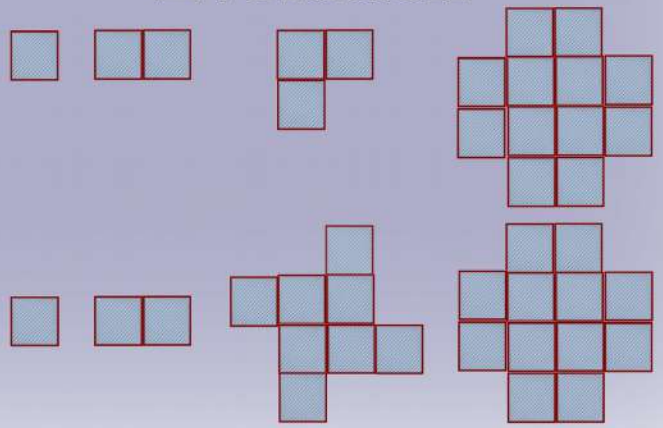
Abstraction



State Space



Evolution



?

Yu Yang Liu

Vibrational frequencies with Quantum Monte Carlo

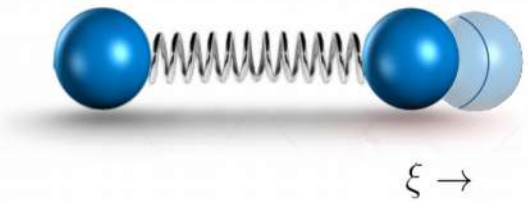
Quantum Monte Carlo

Coupled Cluster

Density Functional Theory

Hartree–Fock

Molecular Dynamics



$$E = \frac{\int \Psi\Psi\frac{H\Psi}{\Psi}\mathrm{d}V}{\int \Psi\Psi\mathrm{d}V} = \left\langle \frac{H\Psi}{\Psi} \right\rangle$$

$$\frac{\partial^2 E}{\partial\xi_i\xi_j} = \left\langle \frac{H''\Psi}{\Psi} \right\rangle + 2\left\langle \frac{\Psi'}{\Psi}\left(\frac{H'\Psi}{\Psi} - \left\langle \frac{H'\Psi}{\Psi} \right\rangle\right) \right\rangle$$

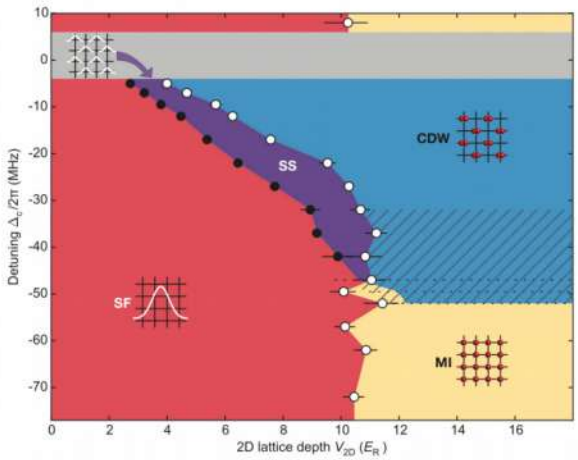
Ezequiel Rodriguez

-Supervisor: Andreas Nunnenkamp

Ultra-cold atoms in optical cavities → Long-range vs. Short-range interactions

$$\hat{H} = -\mu \sum_i \hat{n}_i + \frac{U}{2} \sum_i \hat{n}_i(\hat{n}_i - 1) - t \sum_{\langle i,j \rangle} (\hat{b}_i^\dagger \hat{b}_j + h.c.)$$

$$-\Delta \hat{a}^\dagger \hat{a} + g(\hat{a}^\dagger + \hat{a})(\sum_e \hat{n}_e - \sum_o \hat{n}_o)$$



Esslinger et al.

Dissipation ↔

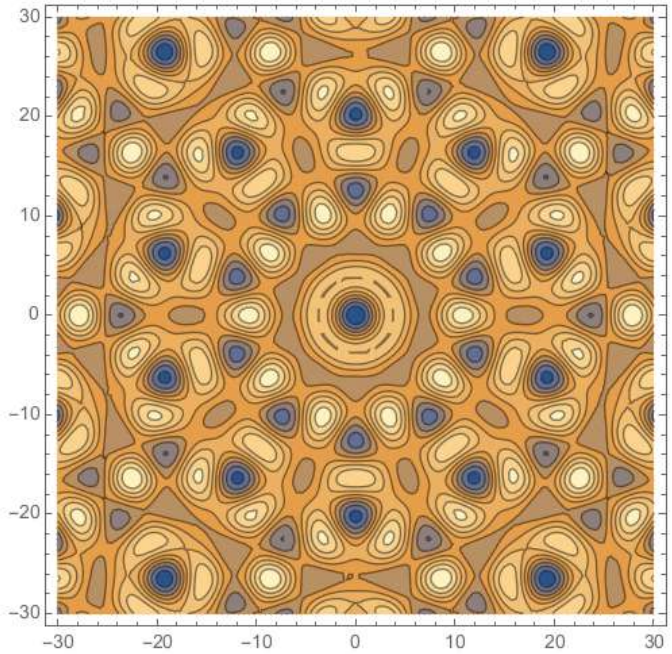
Characterize the system at all time scales!

Accelerating First-Principles Electronic Structure Calculations

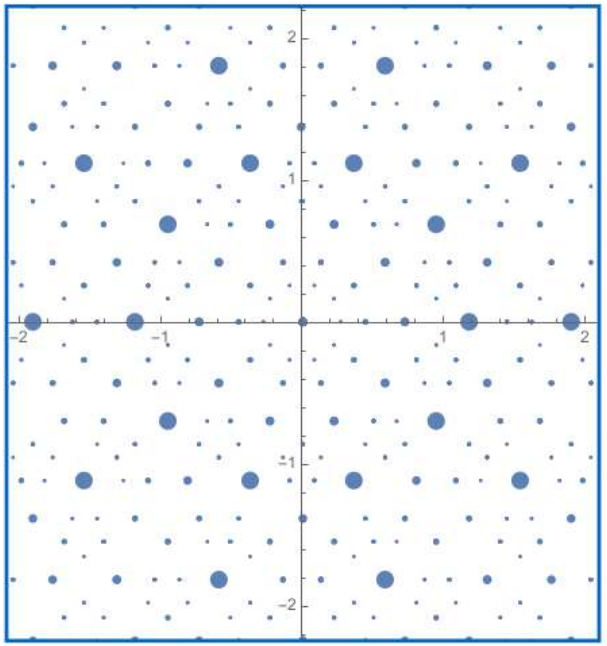
Matthew Smith (mjs281@cam.ac.uk)
Supervisors: Mike Payne & Phil Hasnip

- What?
  - 100k+ cores
  - Emerging computer architectures
- Why?
  - Increase system size
  - Reduce calculation time
- How?
  - Matrix transpositions
    Problems - comms dominated, load balancing issues
    Solutions - new domain decompositions
  - FFTs on GPUs
    x2 speedup - can we do better?
  - Parallel processors
    Problems - ???

Optical Quasicrystals

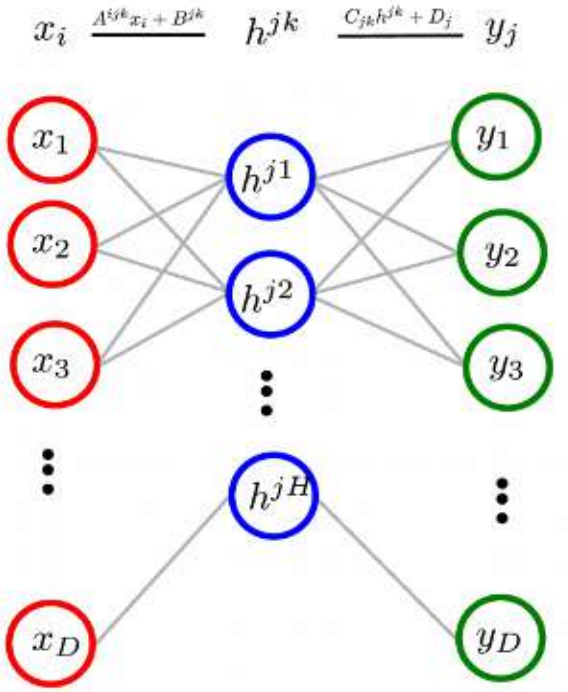


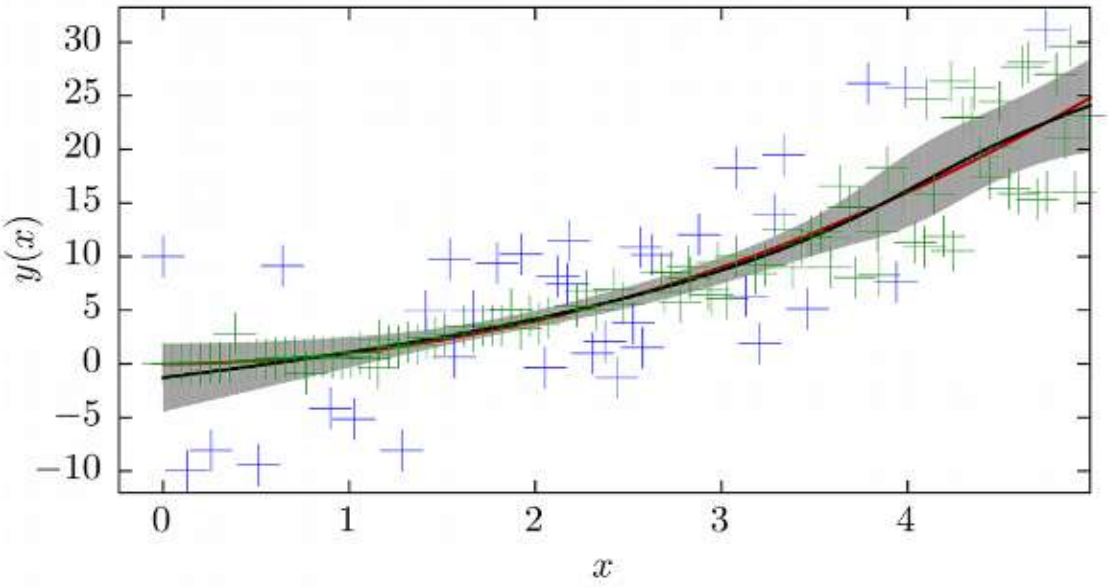
Real Space



Reciprocal Space

$$\epsilon_k a_k + \sum_{k'} V_{kk'} a_{k'} = E a_k$$

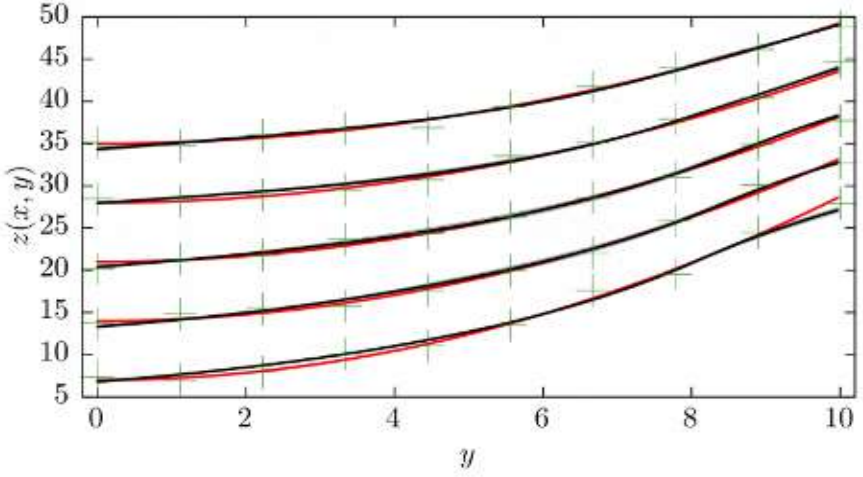


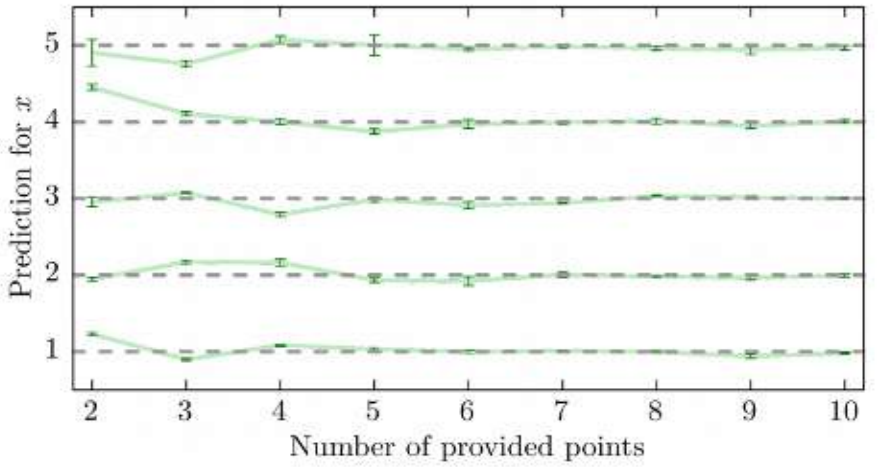


$$f : (x_1, \ldots, x_i, \ldots, x_D) \mapsto (y_1, \ldots, y_j, \ldots, y_D)$$

$$h^{jk} = \tanh\left(A^{ijk}x_i + B^{jk}\right)$$

$$y_j = C_{jk}h^{jk} + D_j$$

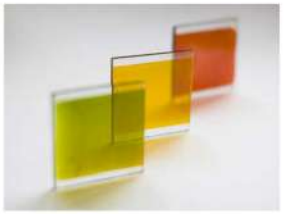




Singlet Fission

Scheme

$$S_1 \longrightarrow T\,T \longrightarrow T_1 + T_1$$



Mechanisms