UNIVERSITY OF CAMBRIDGE

TCM Dragons' Den

Bartholomew Andrews, Kevin Duff, Johannes Hofmann,
Ben Irwin, Victor Jouffrey, Edward Linscott, Tianhan Liu,
Daniel Malz, Paulo Medeiros, Joseph Prentice,
Adam Smith, Philipp Verpoort, & Nathalie Vonrüti

TCM Group, Department of Physics

Rules of the den

Institute of Physics 3 Minute Wonder competition

Talks precisely three minutes long

Maximum of one overhead slide

Running order

Bartholomew Andrews, Kevin Duff, Johannes Hofmann, Ben Irwin, Victor Jouffrey, Edward Linscott, Daniel Malz, Paulo Medeiros, Christopher Parmee, Joseph Prentice, Adam Smith, Philipp Verpoort, and Nathalie Vonrüti

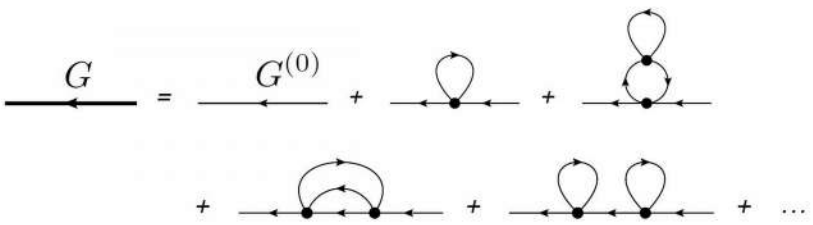
Bartholomew Andrews

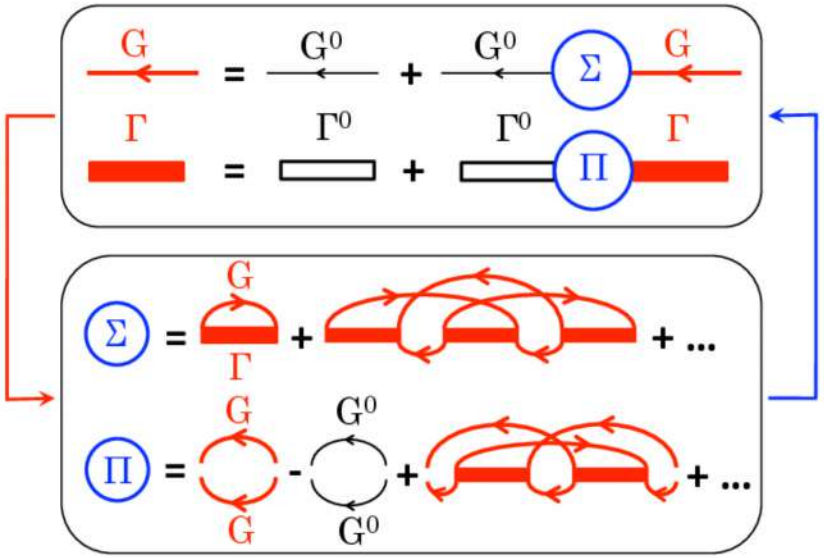
Bold Diagrammatic Monte Carlo

Monte Carlo → diagMC → BDMC

single-particle propagator

$$G_\sigma(\mathbf{p},\tau) = -\left\langle \mathrm{T}\ \hat{c}_{\mathbf{p},\sigma}(\tau)\hat{c}^\dagger_{\mathbf{p},\sigma}(0)\right\rangle$$





Kevin Duff

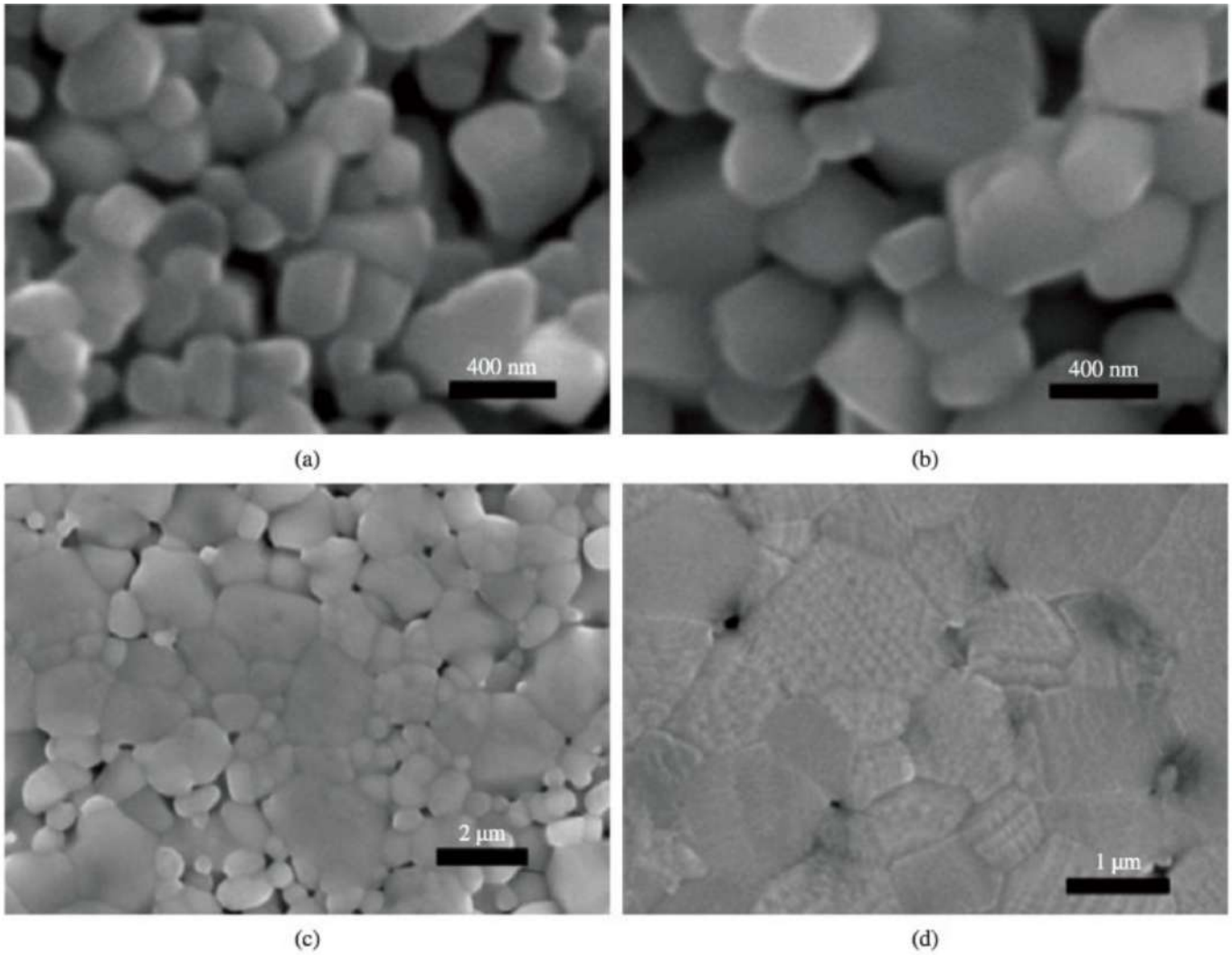
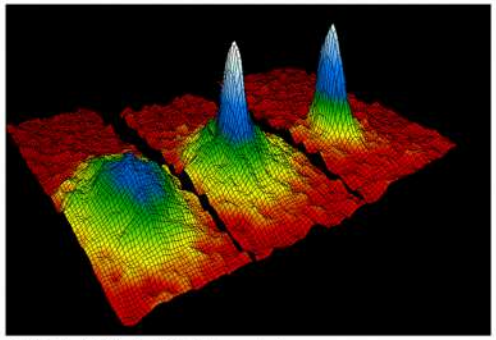


Figure 2. SEM surface images of Ni-ferrite sintered for 4 hours at: a) 1000 °C; b) 1100 °C; c) 1150 °C; and d) 1200 °C. Source: F. L. Zabotto et al.

Damping of bright solitons in Bose-Einstein condensates

J. Hofmann + D. Efimkin, V. Galitski



NIST/JILA/CU-Boulder

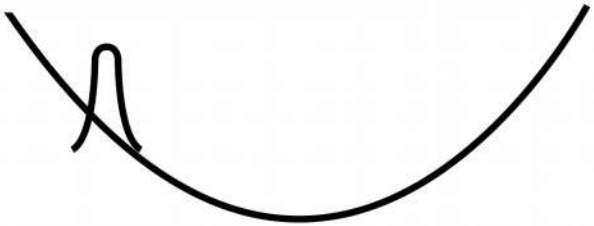
1D attractive interaction: bright soliton

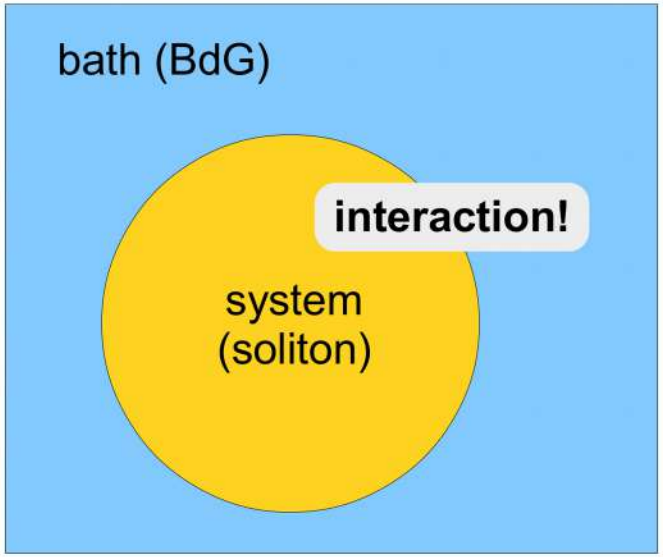
$$\phi(x,t) = \phi_0(x) + \delta\phi(x,t)$$

Elementary excitations: Bogoliubov-deGennes

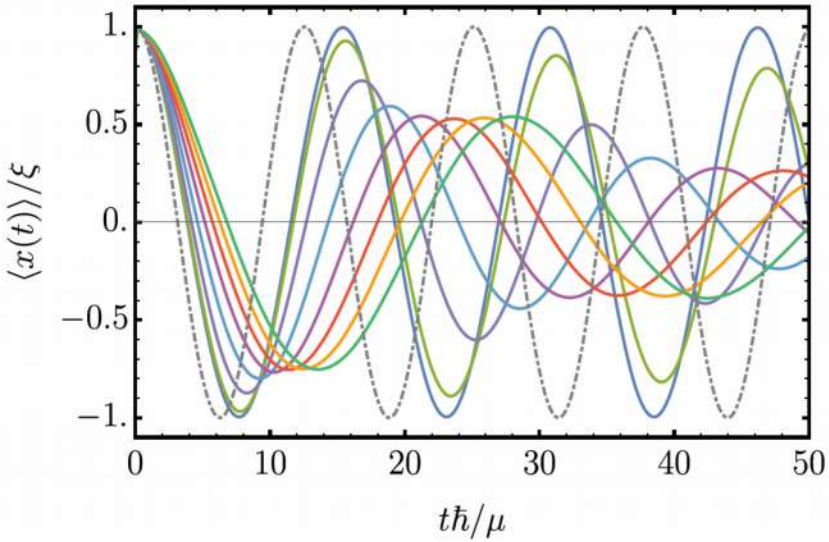
Gross-Pitaevskii

$$\left[-\frac{\hbar^2\nabla^2}{2m} - \mu + g_1|\phi_0(x)|^2\right]\phi_0(x) = 0$$





Quantum dissipation of soliton motion

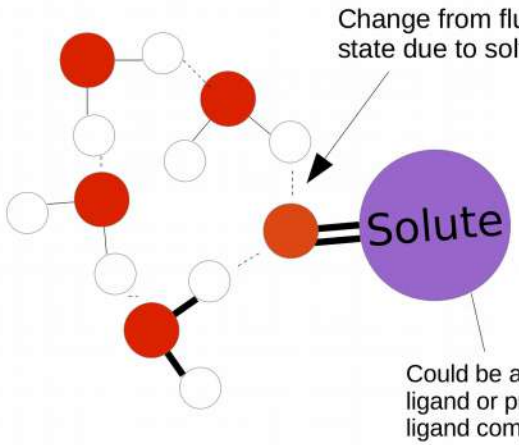


Benedict Irwin

Measuring Solvation Entropy with Inhomogeneous Fluid Solvation Theory

- Binding affinity
- Protein Druggability
- Structure of Water

Free Energy of Solvation



corresponding change in n-body correlation functions

$$g^{(n)}(\vec{r}_1, \cdots, \vec{r}_n, \vec{\omega}_1, \cdots, \vec{\omega}_n)$$

$$S = s_{id} + \frac{1}{\Omega}\int_V g^{(2)}\ln g^{(2)}\, d\vec{r}_1 d\omega + \frac{\rho}{2\Omega^2}\iint_V g^{(3)}\ln g^{(3)}\, d\vec{r}_1 d\vec{r}_2 d\omega_1 d\omega_2 + \cdots$$

Cluster Expansion: 1-body, 2-body, ...

K-Nearest Neighbours

$$I = \int_{R^s} f(\vec{x})\ln f(\vec{x})\, d\vec{x}$$

$$I \approx \frac{1}{N}\sum_{i=1}^{N} \ln\left(\frac{N d_{i,k}^s \pi^{s/2}}{\Gamma(\frac{s}{2}+1)}\right) - \psi(k)$$

- Run MD simulations, collect data
- Find nearest neighbours
- Estimate entropy change
- Compare free energy to FEP

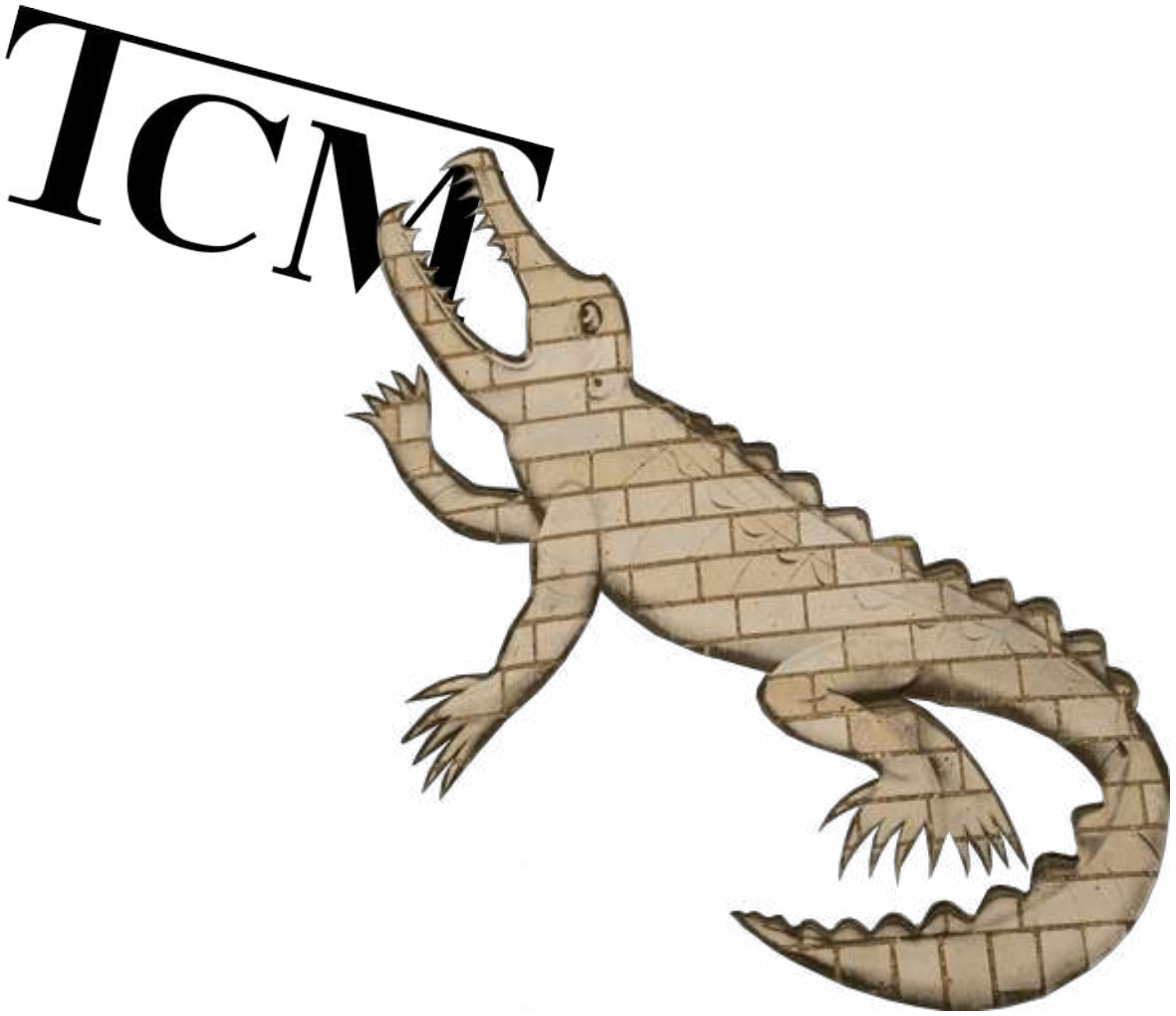
- Allows a spatial distribution of entropy change

- How much does the 2 body term contribute?

- Fixed bond, unfixed bond differences?

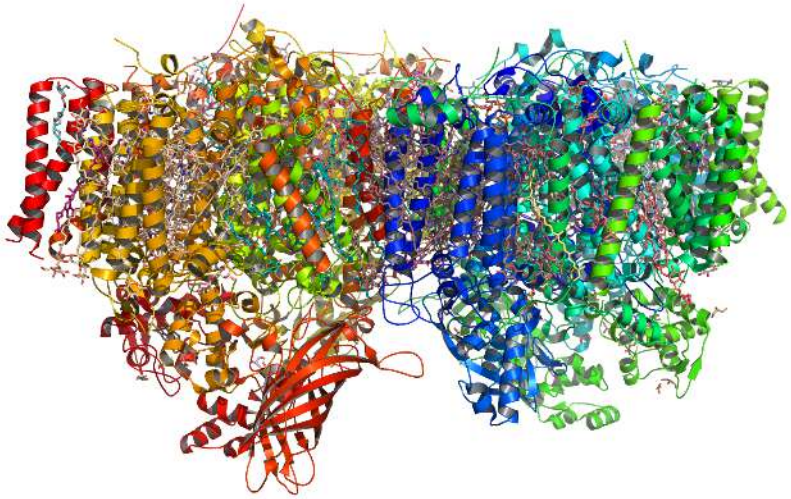
EPSRC Centre for Doctoral Training | Computational Methods for Materials Science

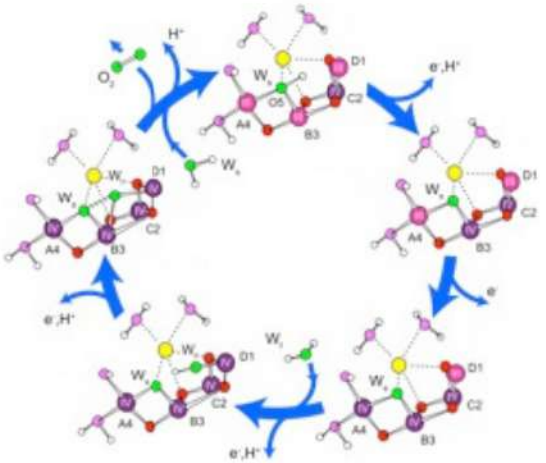
Victor Jouffrey

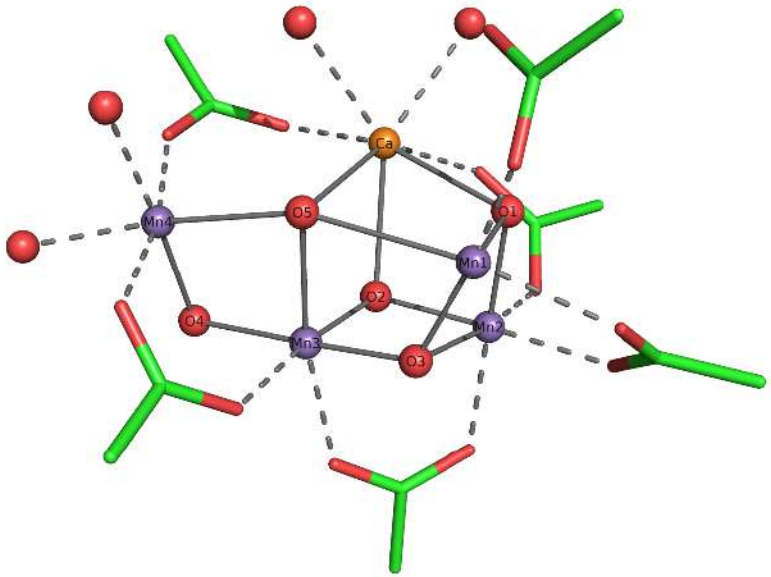


Strongly-correlated electrons in biology

Edward Linscott (Supervisor: Danny Cole)





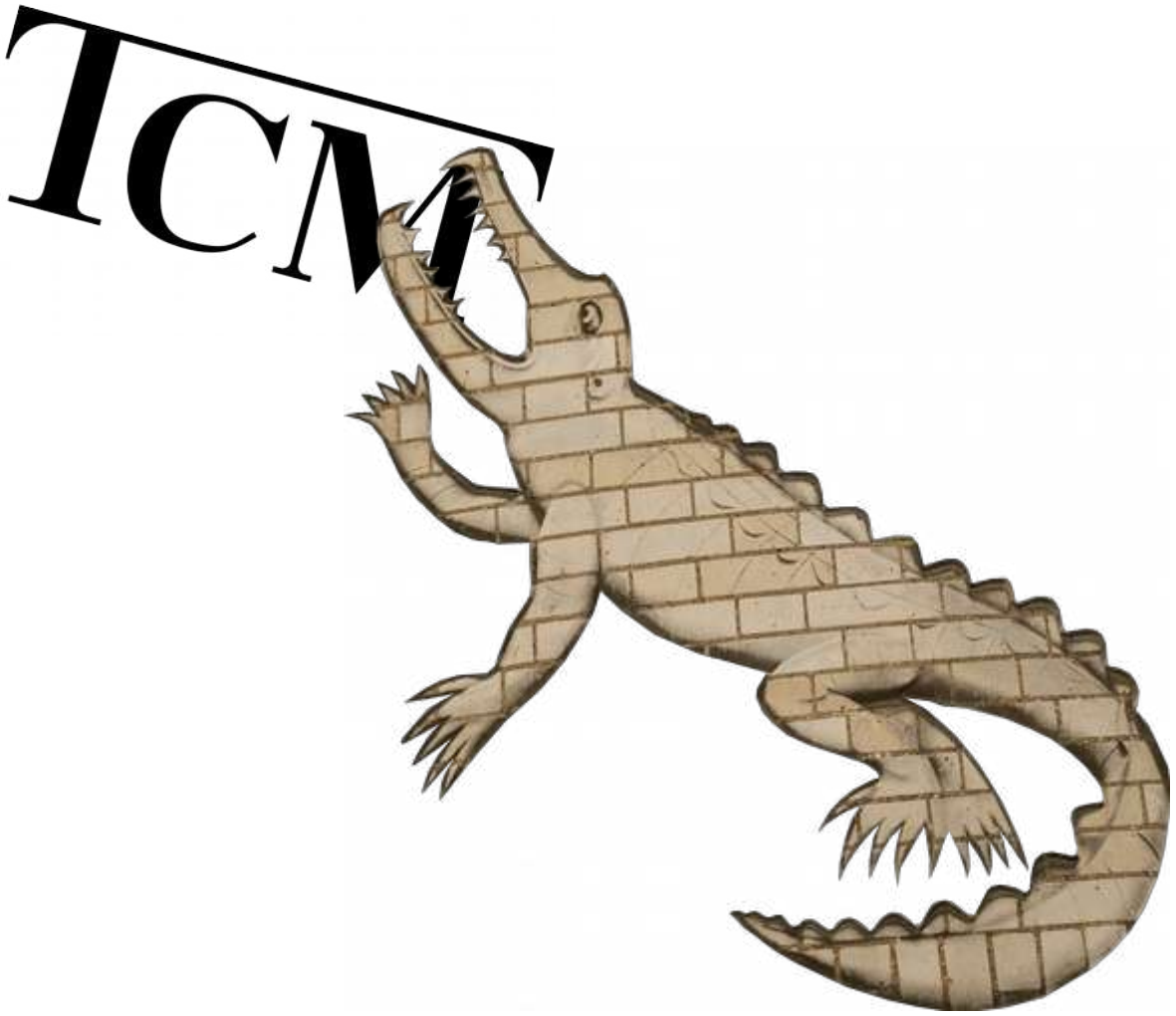


$$2\mathrm{H_2O} + h\nu \rightarrow 4\mathrm{H^+} + 4e^- + \mathrm{O_2}$$

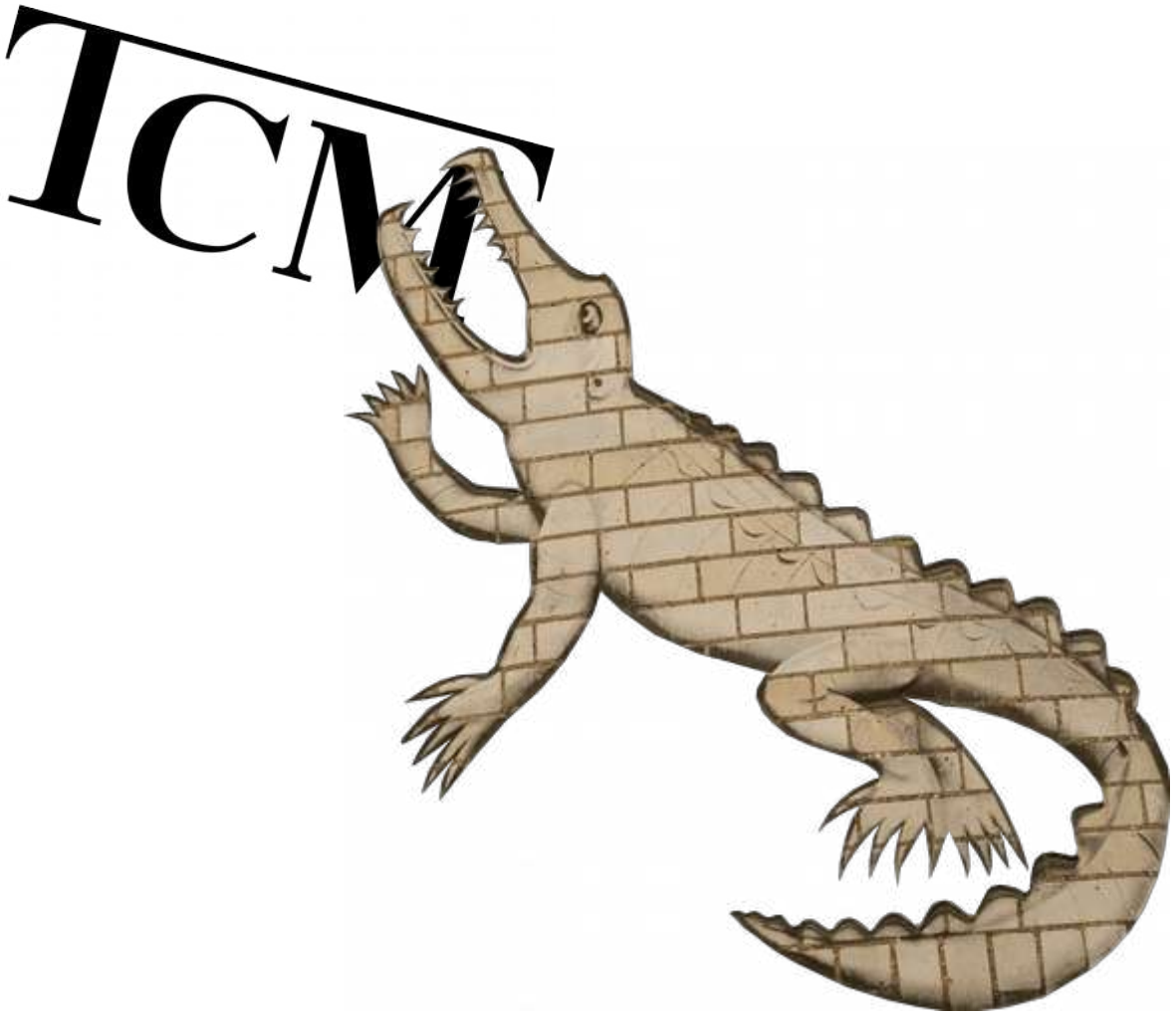
Need to carefully treat...

- surrounding protein (ONETEP)
- correlation (DFT + U, DMFT)

Tianhan Liu



Daniel Malz



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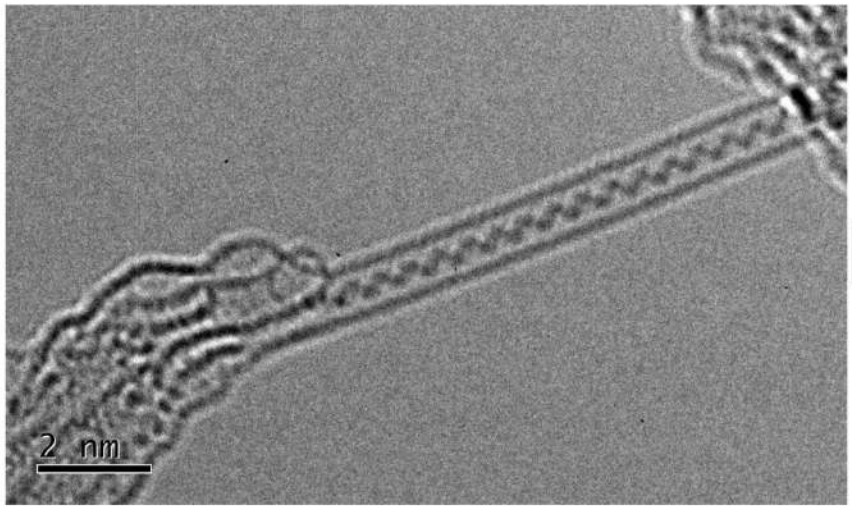
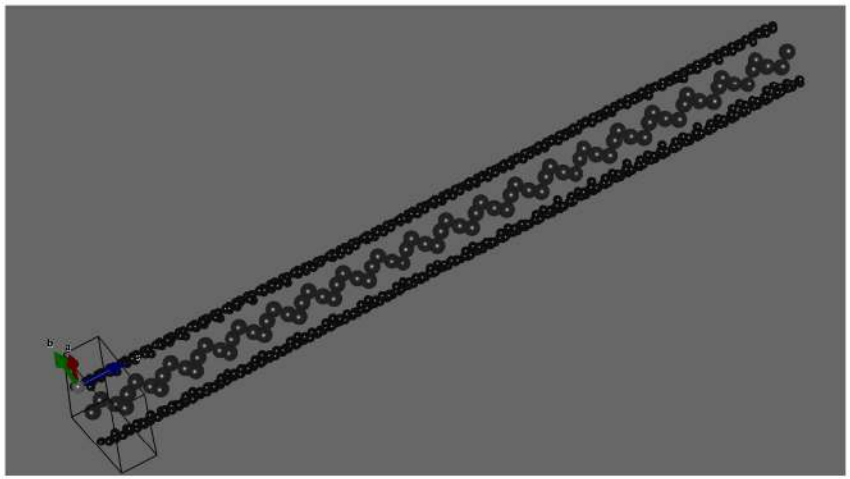




Modelling nanowires encapsulated inside CNTs

Paulo V. C. Medeiros

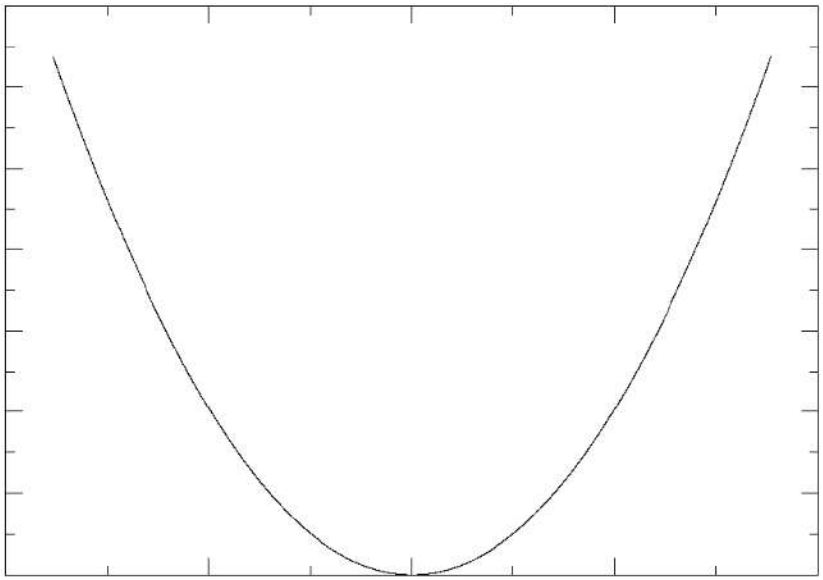
University of Cambridge

"Dragons' Den" TCM seminar, 26 November 2015

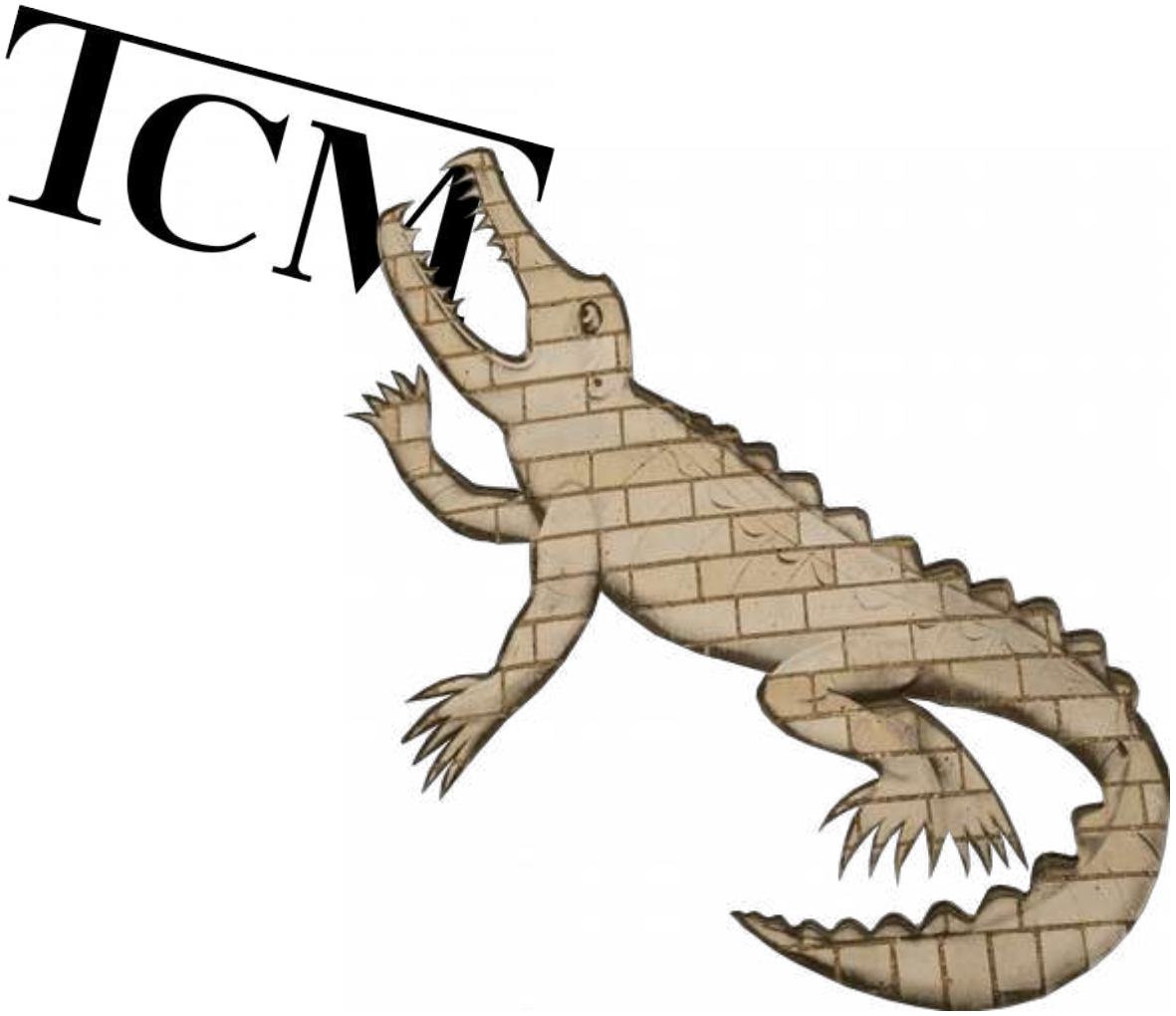
TCM Dragon's Den

J.C.A. Prentice

- Nuclear equation of motion: $(T_n + E_{el}(\mathbf{R}))\psi_n = E_n\psi_n$
- Vibrational self-consistent field equation: $(-\frac{1}{2}\frac{\partial^2}{\partial q_{n\mathbf{k}}^2} + \bar{V}_{n\mathbf{k}}(q_{n\mathbf{k}}))|\phi_{n\mathbf{k}}\rangle = \lambda_{n\mathbf{k}}|\phi_{n\mathbf{k}}(q_{n\mathbf{k}})\rangle$

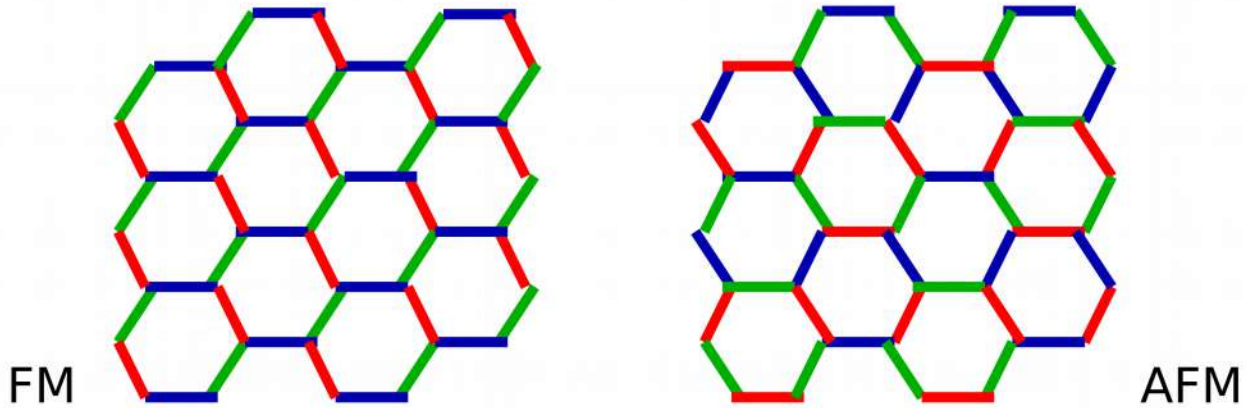


Adam Smith

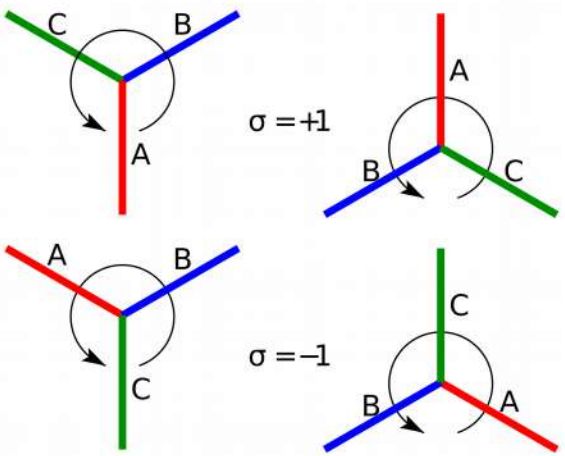


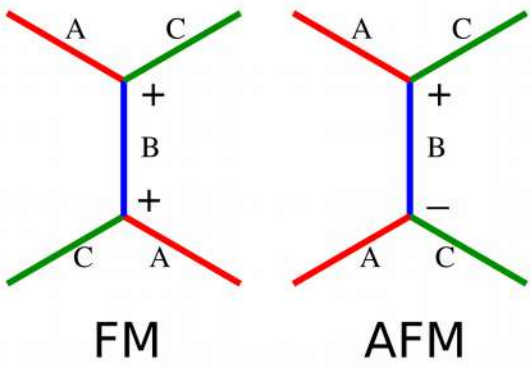
Philipp Verpoort, from Karlsruher Institute of Technology (KIT) in Germany,
Masterthesis with Claudio Castelnovo on

"Colour-dependent Interactions in the Three-colouring Model"



$$H = -J_{\mathrm{A}} \sum_{\langle ij \rangle_{\mathrm{A}}} \sigma_i \sigma_j - J_{\mathrm{B}} \sum_{\langle ij \rangle_{\mathrm{B}}} \sigma_i \sigma_j - J_{\mathrm{C}} \sum_{\langle ij \rangle_{\mathrm{C}}} \sigma_i \sigma_j$$

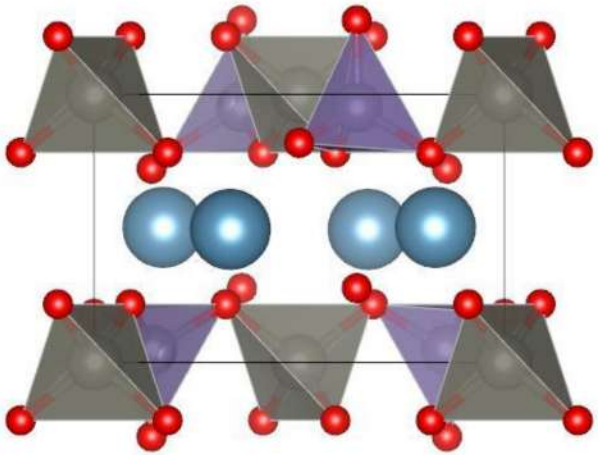




Electronic structure prediction of magnesium-ion battery materials

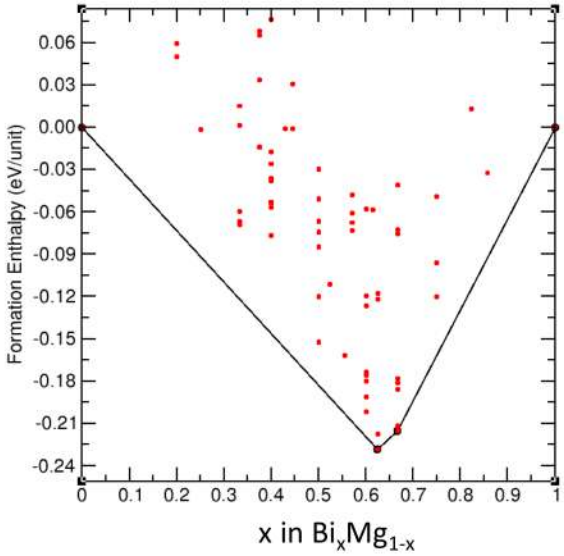
Main challenge: diffusion of Mg^{2+}

Cathode



Mg_2FeSi_2O7

Anode



Bi_xMg_y

Nathalie Vonrüti