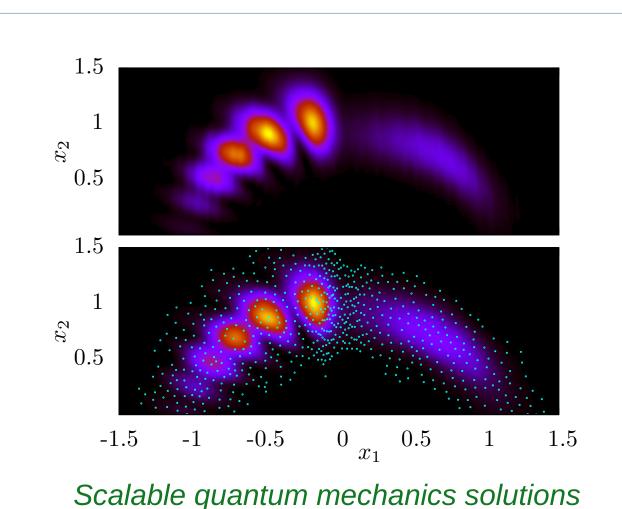


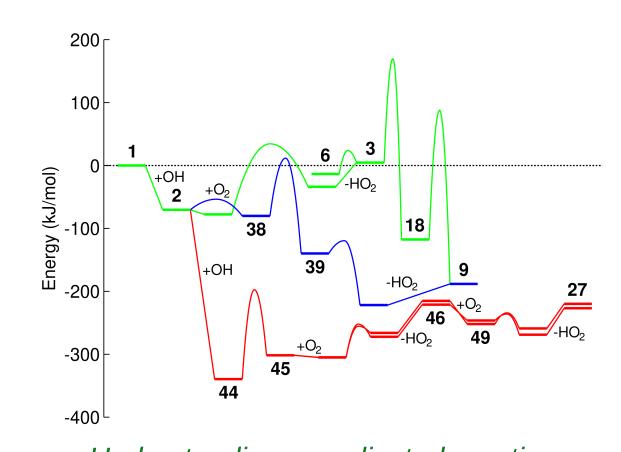
Molecular and materials modelling

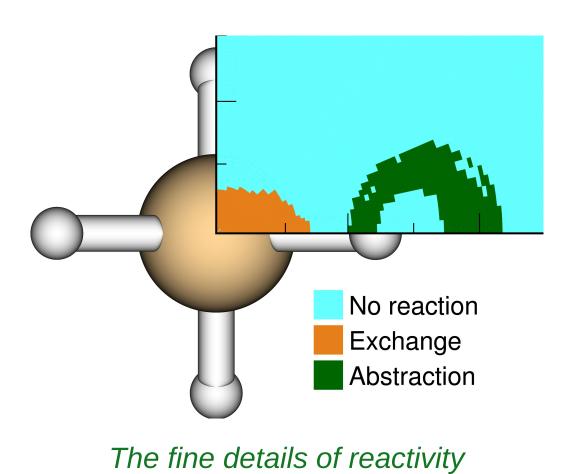
Terry Frankcombe

Molecules

- Potential energy surface interpolation
- Molecular dynamics for reactions
- Quantum dynamics method development



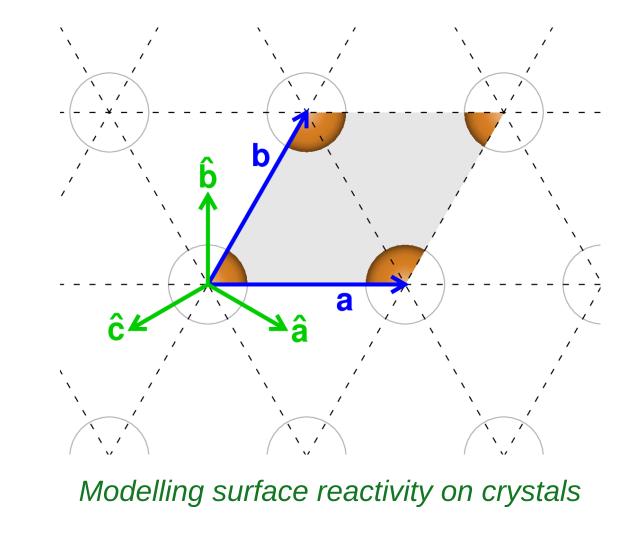


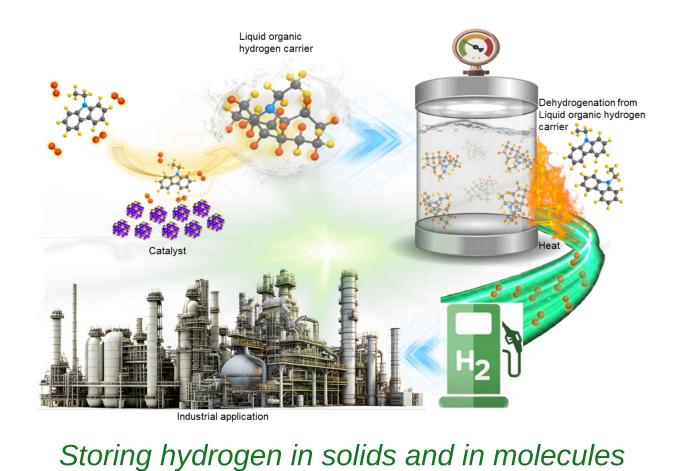


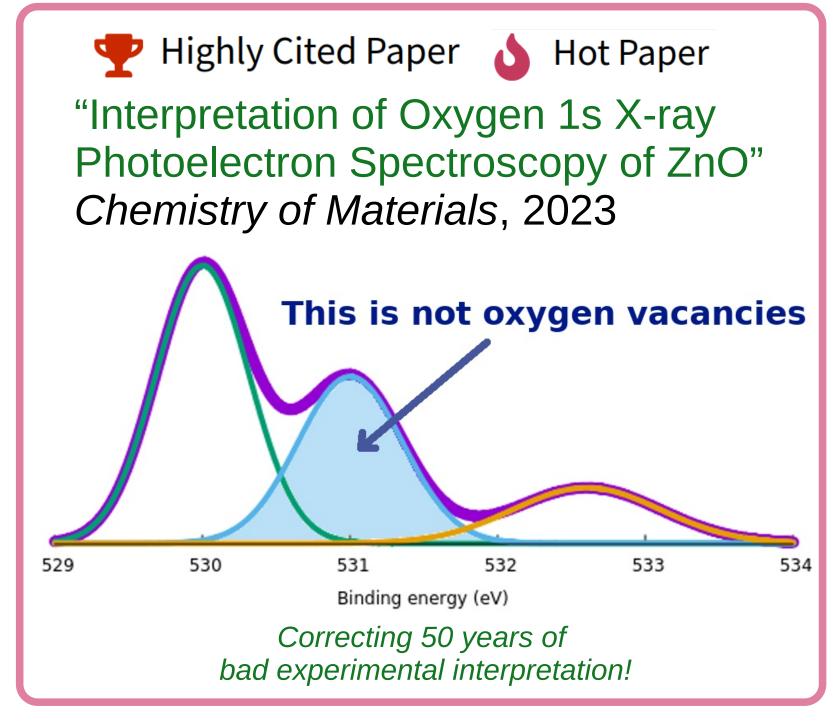
Understanding complicated reactions

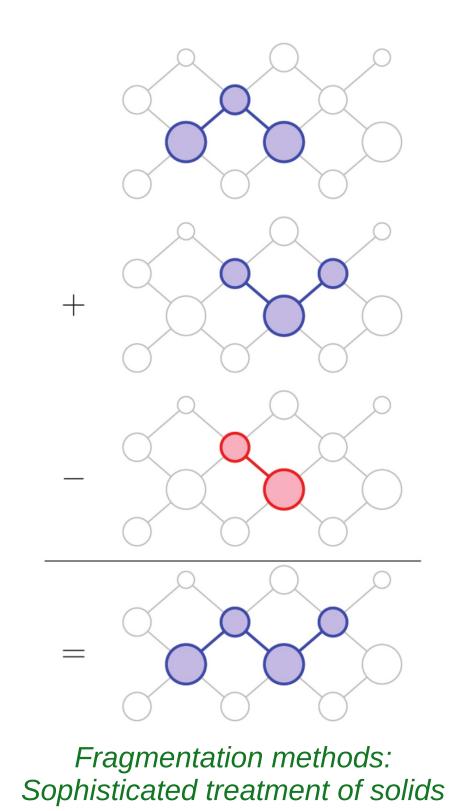
Multiscale applications

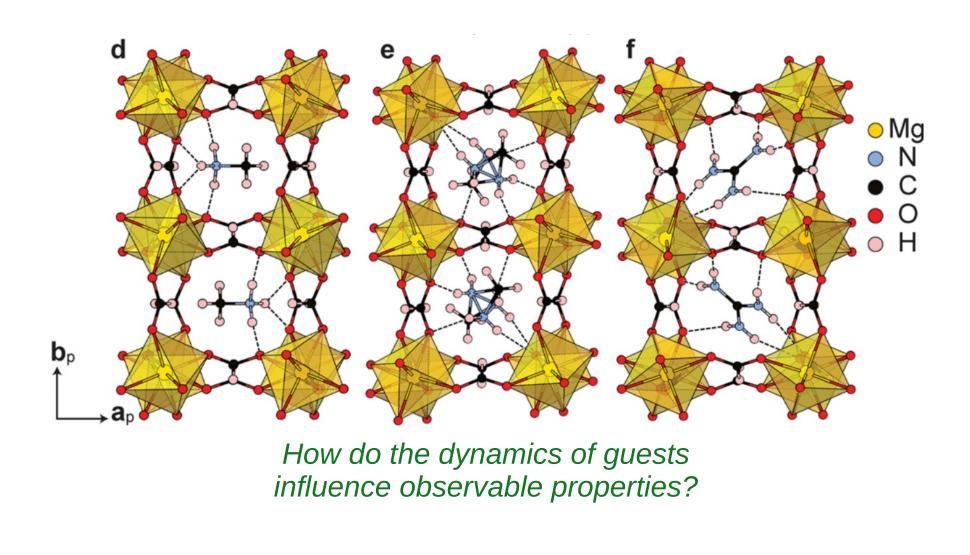
- Hydrogen storage
- Gas-surface reactions
- Fragmentation methods
- Interstellar chemistry
- Ion thruster chemistry
- Host-guest systems

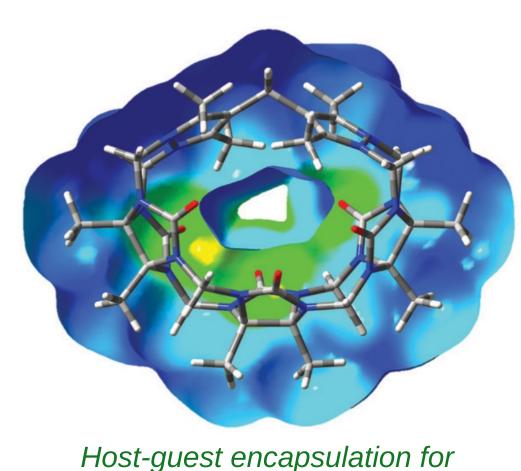




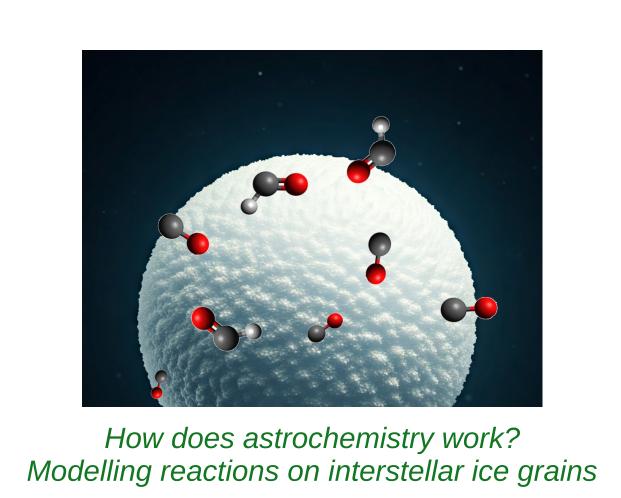




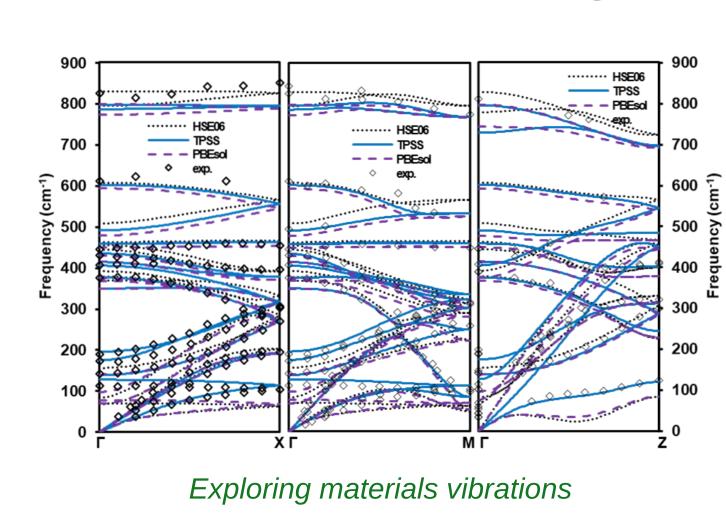




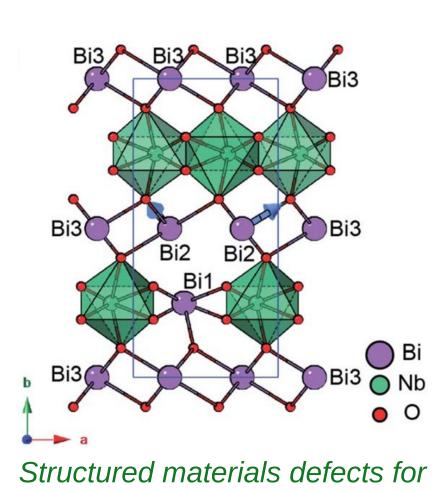
applications like drug delivery



DFT modelling

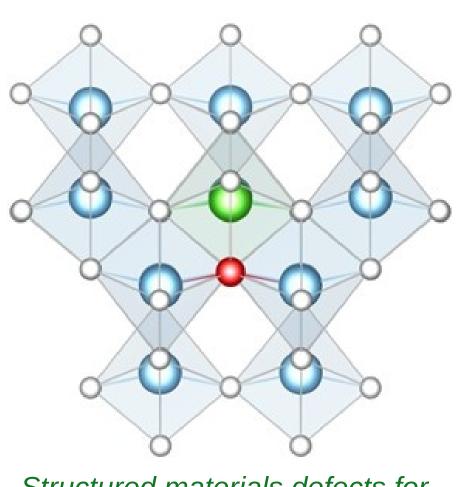


Dielectric properties

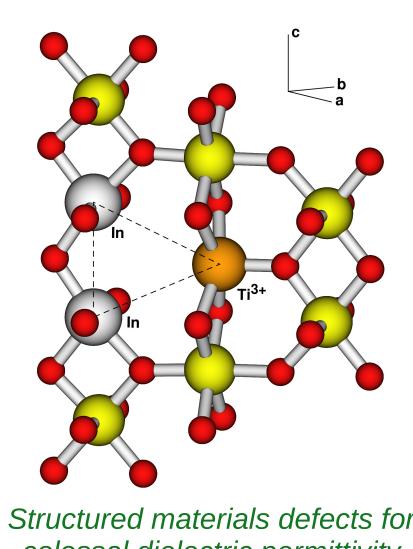


photovoltaic films

Ferroelectrics/mutiferroics

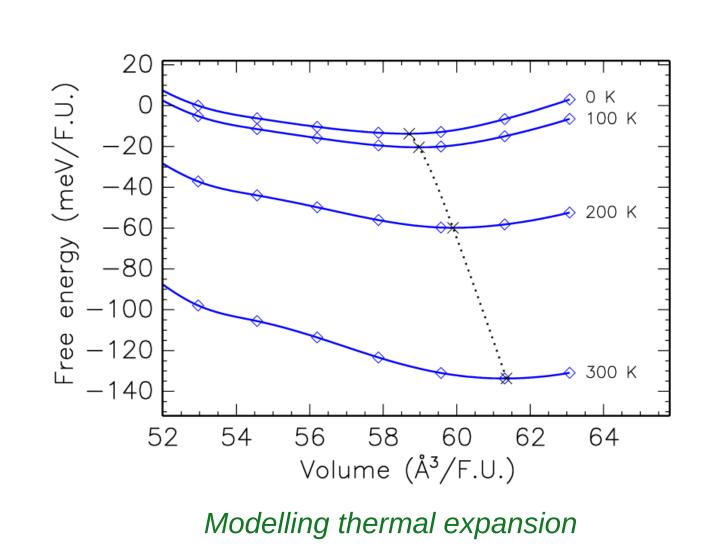


Structured materials defects for visible light catalysis



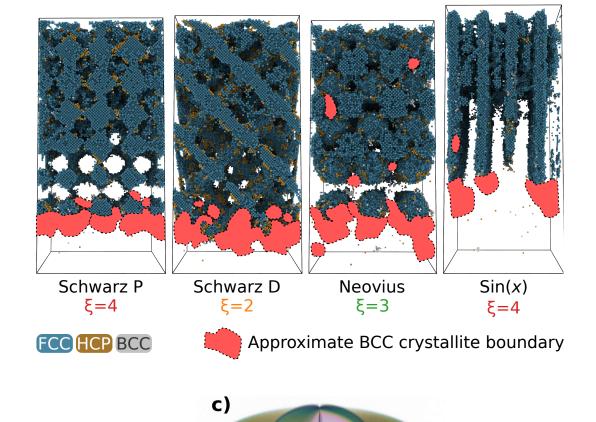
Structured materials defects for colossal dielectric permittivity

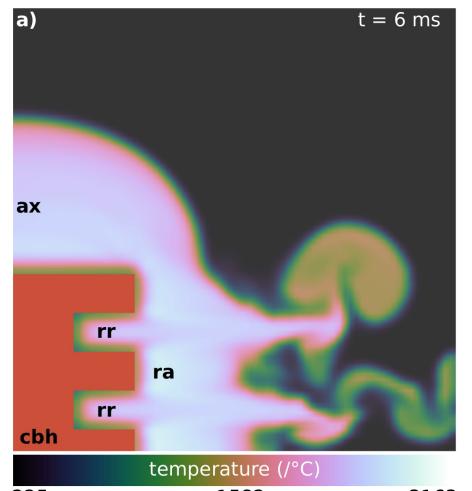
Photocatalysis

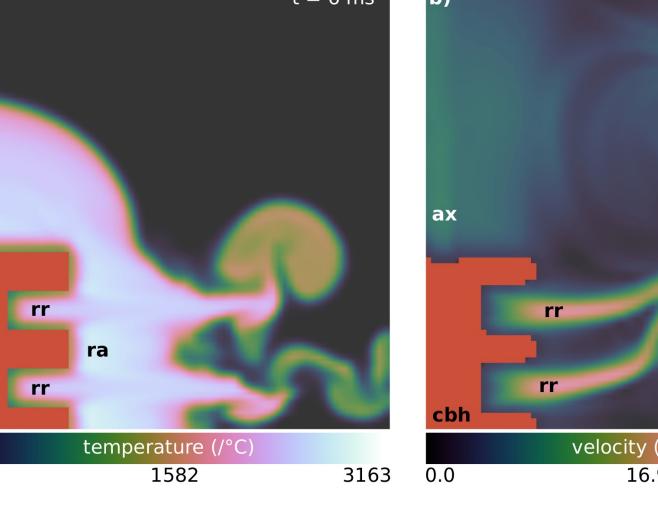


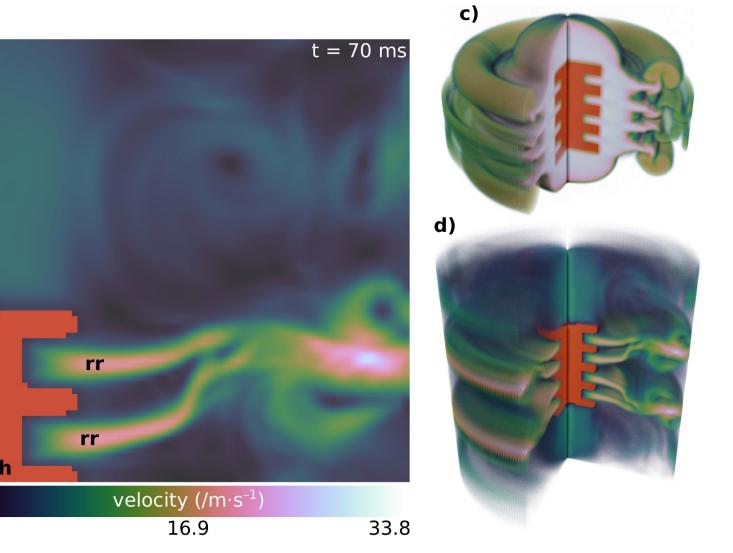
Energetic materials

- Reactive materials
- Effect of shape on combustion
- Rocketry



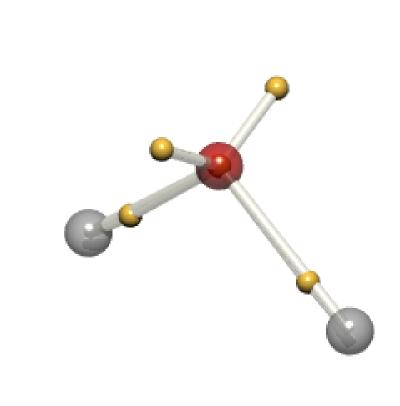


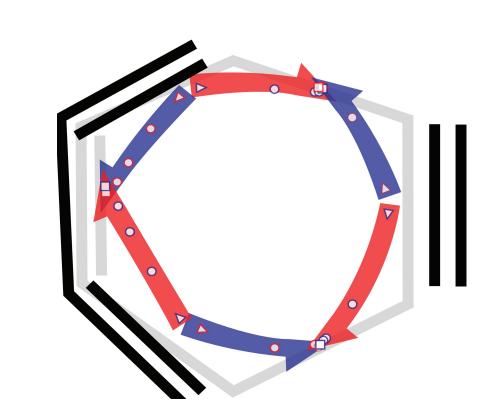


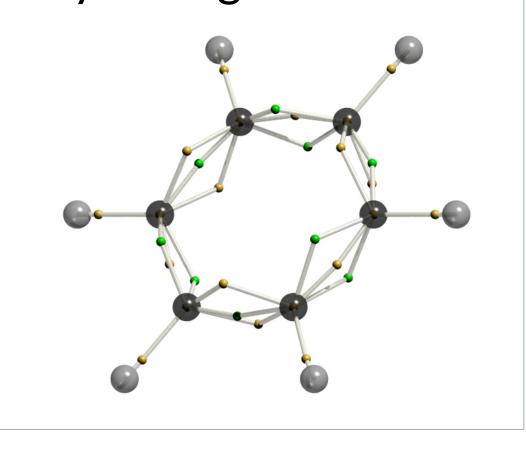


Fundamental theory

 Dynamic Voronoi Metropolis Sampling: What are multielectron wavefunctions actually telling us?







Funding

- ARC Discovery Projects
- ARC Linkage Project
- Department of Defence