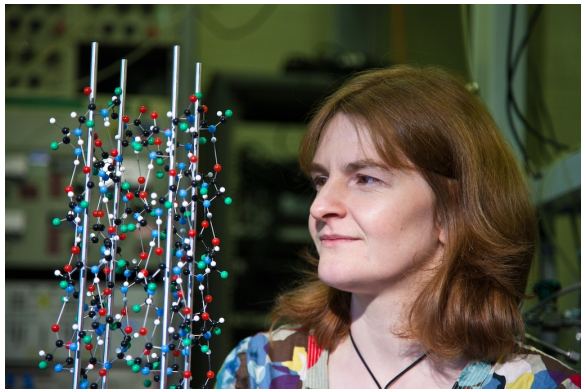
Molecular Dynamics Simulations in the School of Chemistry

Philip Camp

Fernanda Duarte

Adam Kirrander

Julien Michel



Carole Morrison

Research themes

1. **Reaction dynamics and electron/X-ray scattering**
   Adam Kirrander

2. **Solid-state structure and dynamics**
   Carole Morrison

3. **Catalysis**
   Fernanda Duarte

4. **Molecular liquids and biomolecular systems**
   Philip Camp, Julien Michel, Carole Morrison

5. **Soft matter**
   Philip Camp

Simulation methods

1. **Few-atom quantum dynamics**
   Adam Kirrander

2. **Ab-initio and Car-Parrinello molecular dynamics**
   Carole Morrison

3. **Quantum mechanics/molecular mechanics**
   Fernanda Duarte

4. **Classical atomistic molecular dynamics**
   Philip Camp, Julien Michel, Carole Morrison

5. **Coarse-grained dynamics**
   Philip Camp

length/time

1. Adam Kirrander: Reaction dynamics

- **Few-atom quantum dynamics**
  Andrés Moreno, Darren Bellshaw, Nikola Zotev, Maria Tudorovskaya, and Minas Stefanou

archer LCLS The Leverhulme Trust THE CARNEGIE TRUST FOR THE UNIVERSITIES OF SCOTLAND MARIE CURIE ACTIONS

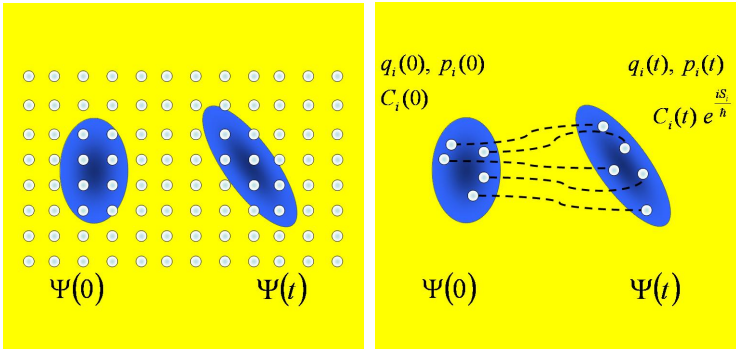
1. Adam Kirrander: Reaction dynamics

- Interpreting ultrafast X-ray (XFEL) and electron diffraction measurements to generate 'molecular movies'

scattering theory

grid-based methods
$N \lesssim 20$ atoms

semi-classical dynamics



$$\hbar \to 0$$

$$\Psi = \sum_k c_k g_k(\bar{\boldsymbol{q}}_t, \bar{\boldsymbol{p}}_t)$$

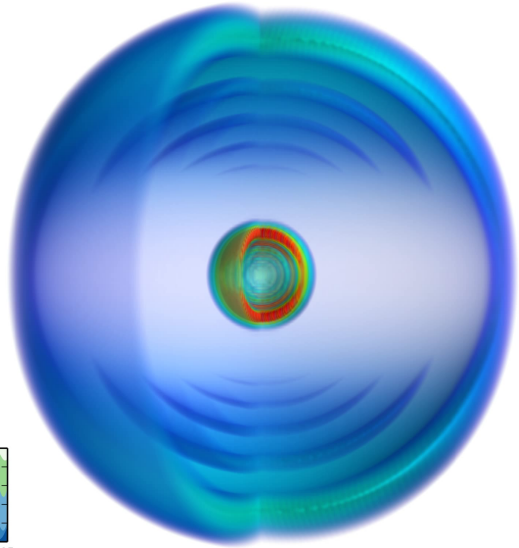
accuracy

number of atoms

1. Adam Kirrander: Reaction dynamics

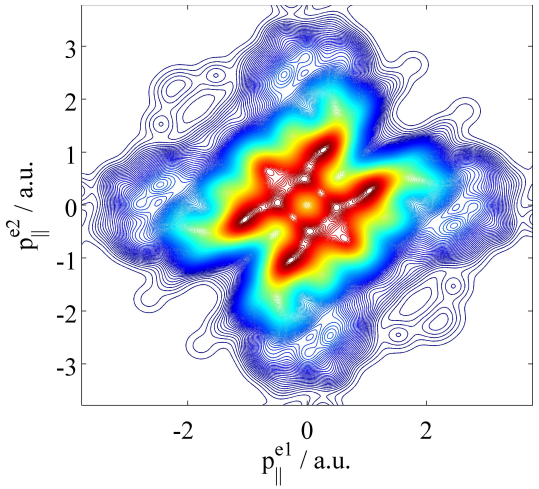
Electron dynamics in argon

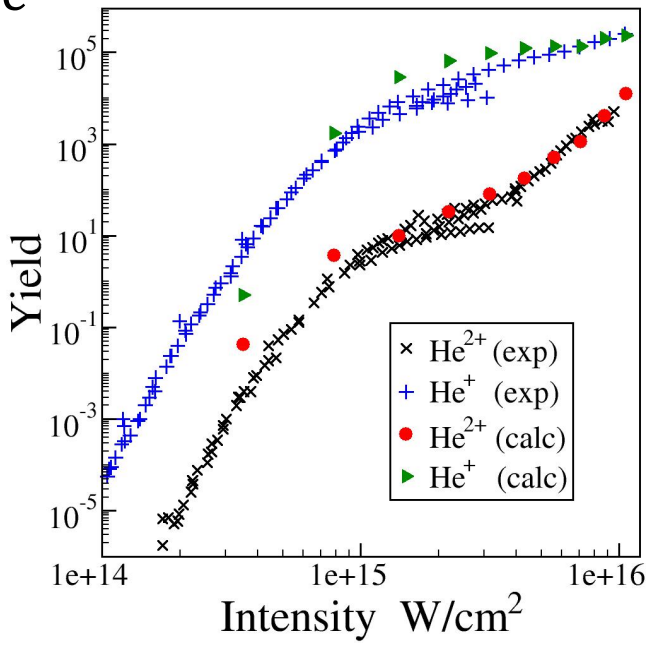
Phys. Rev. Lett. **112**, 043002 (2014)

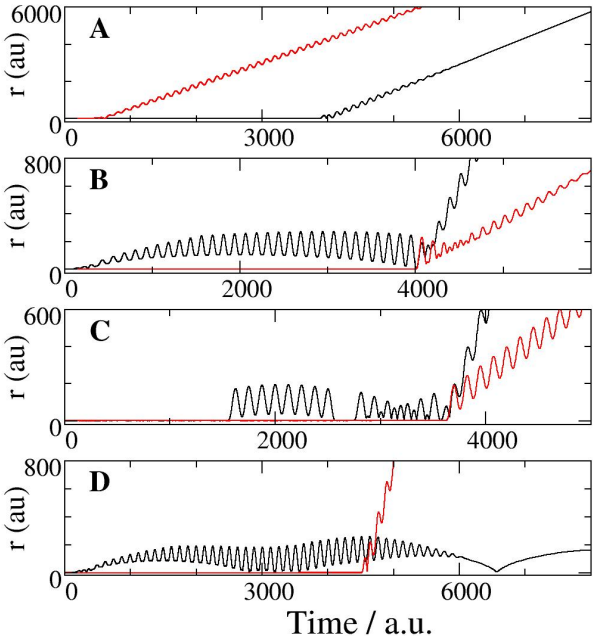


Double ionisation of He

Phys. Rev. A **84**, 033406 (2011)





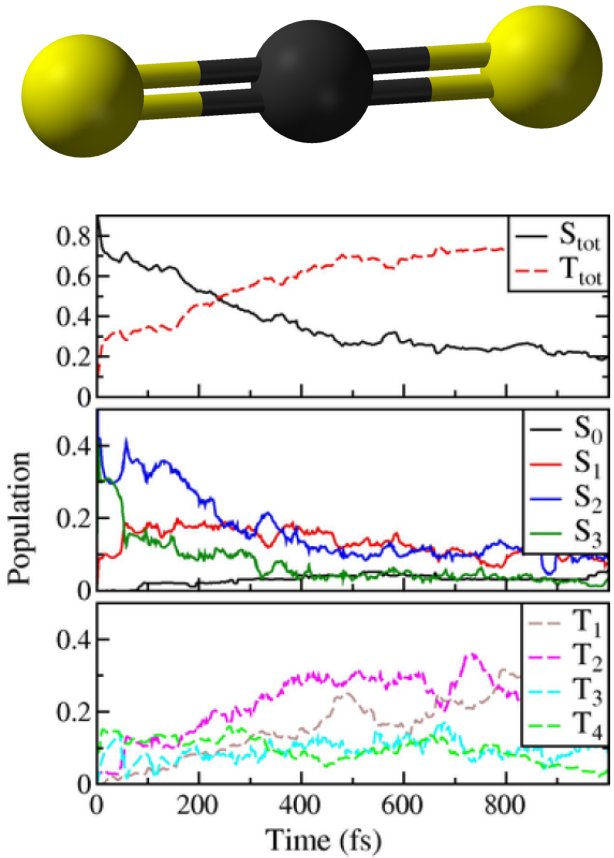


1. Adam Kirrander: Reaction dynamics

Efficient dissociation of CS_2 promoted by spin-orbit coupling

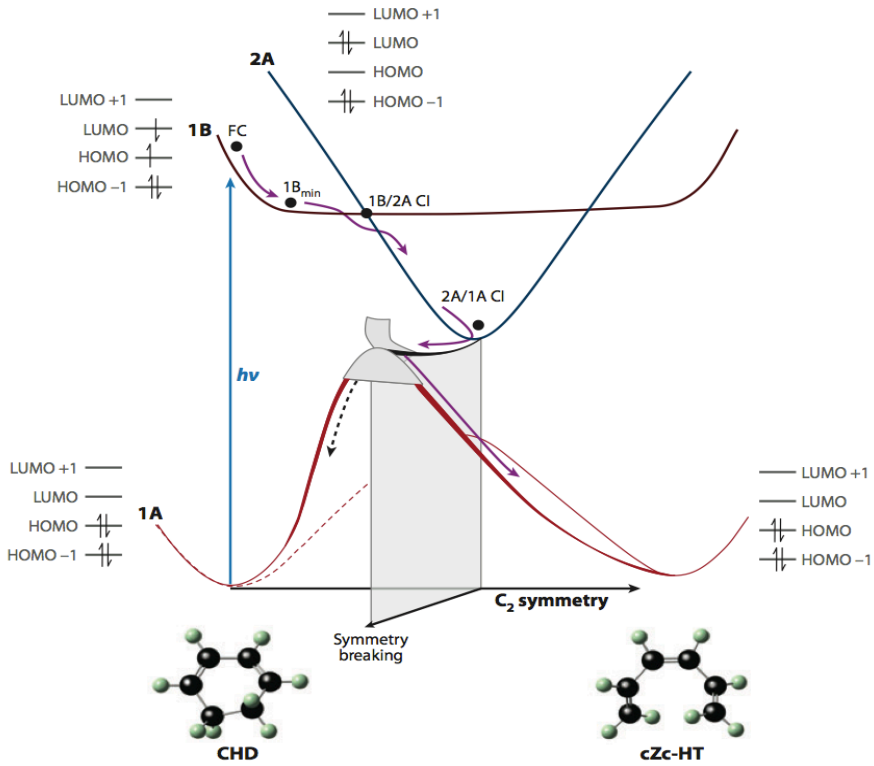
$CS_2 + h\nu \rightarrow CS(X) + S(^1D_1 \text{ or } ^3P)$

Chem. Phys. Lett. (in press)



1,3-cyclohexadiene ring-opening

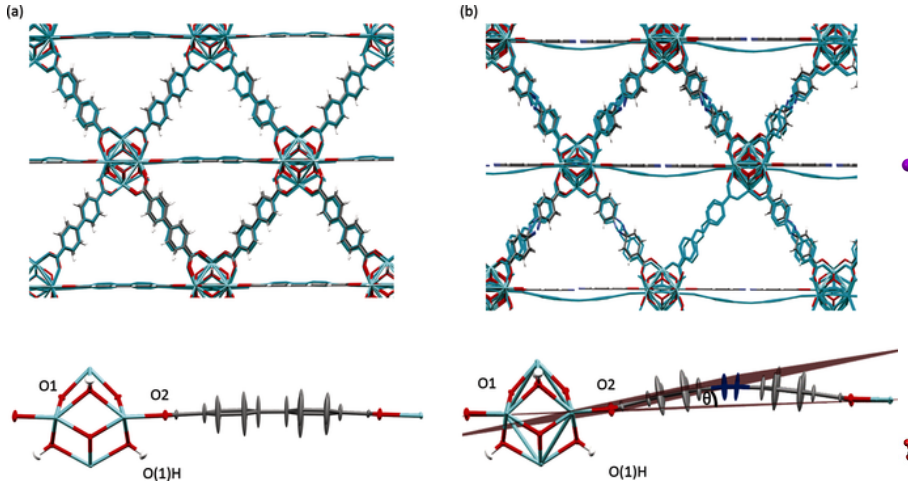
Phys. Rev. Lett. **114**, 255501 (2015)

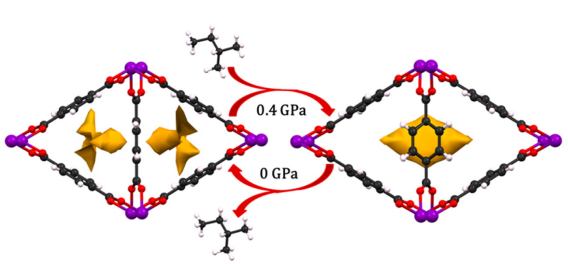


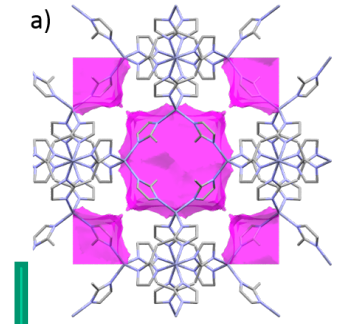
2. Carole Morrison: Solid-state structure and dynamics

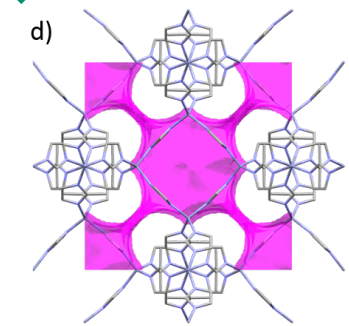
- **Ab-initio and Car-Parrinello molecular dynamics**
  Stephen Moggach, Tina Düren, Claire Hobday, and Jonathan Richardson

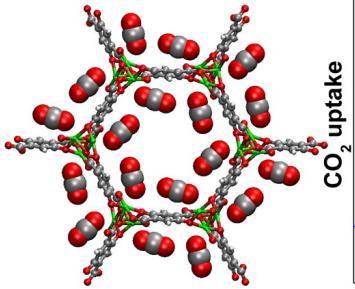
- Combining experiment and theory to understand solid-state structure, reaction dynamics, and adsorption of small molecules (CO_2, H_2, etc.)

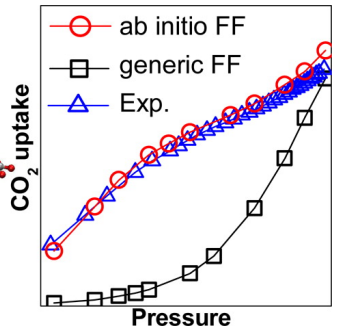










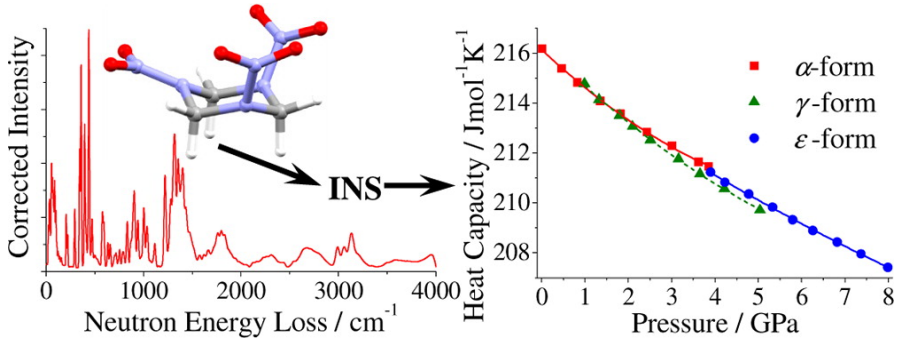


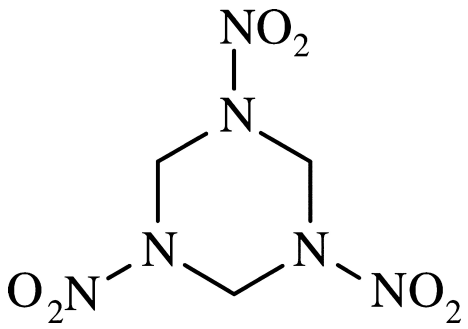
J. Am. Chem. Soc. **135**, 15763 (2013)
Angew. Chem. Int. Ed. **128**, 2447 (2016)
Chem. Mater. **28**, 466 (2016)
Nature Chem. (in press)

2. Carole Morrison: Solid-state structure and dynamics

- **Ab-initio and Car-Parrinello molecular dynamics**
  Colin Pulham and Adam Michalchuk

- Predicting impact sensitivities of energetic materials from first-principles phonon calculations



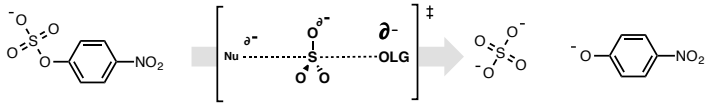


J. Phys. Chem. C **119**, 2322 (2015)

3. Fernanda Duarte: Catalysis

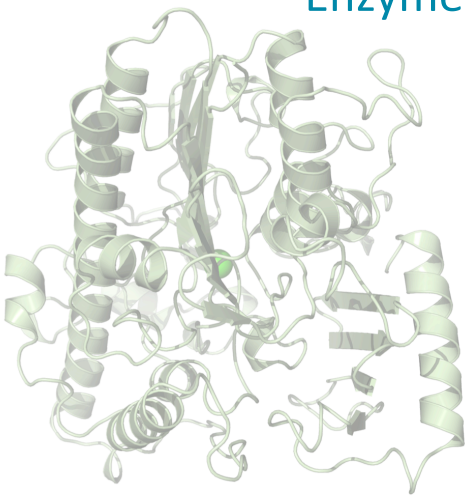
- **Quantum mechanics/molecular mechanics**

BBA – General Subjects **1850**, 954 (2015)



Reaction Mechanism

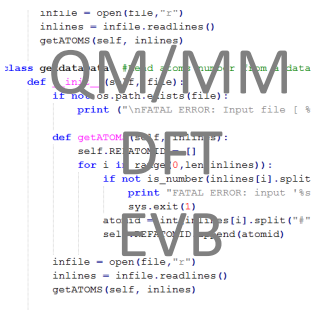
Enzyme Catalysis



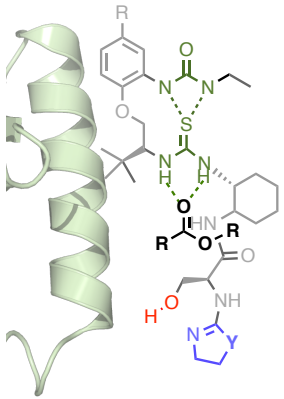
QM/MM

DFT

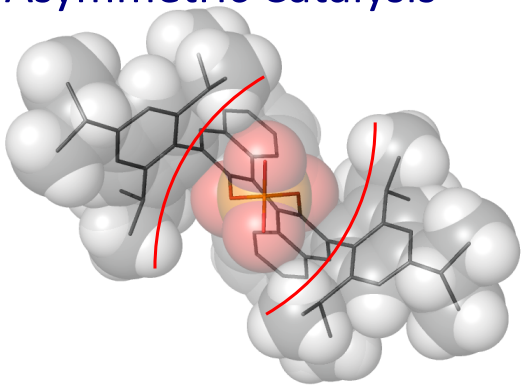
EVB



Biomimetic Catalysis

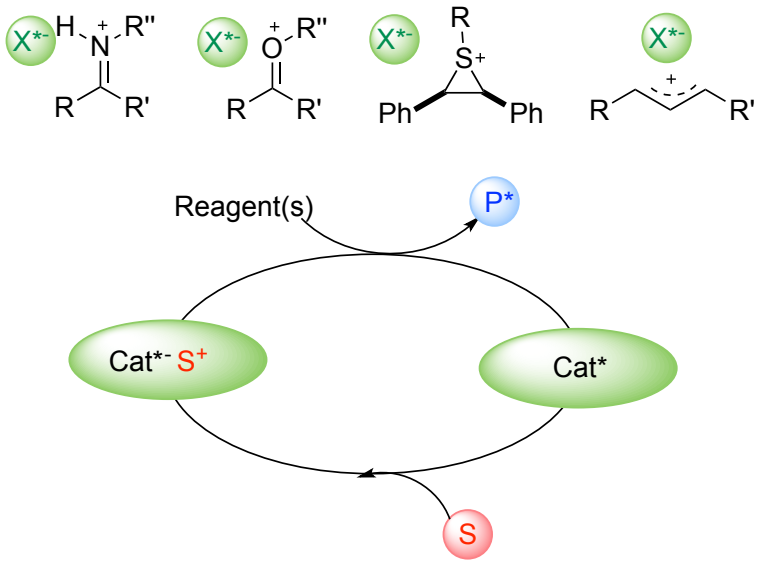


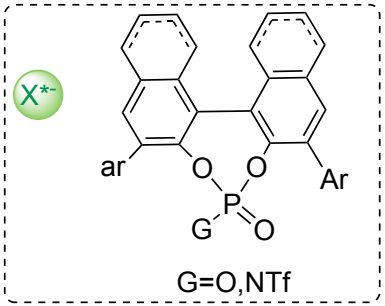
New Models for Asymmetric Catalysis

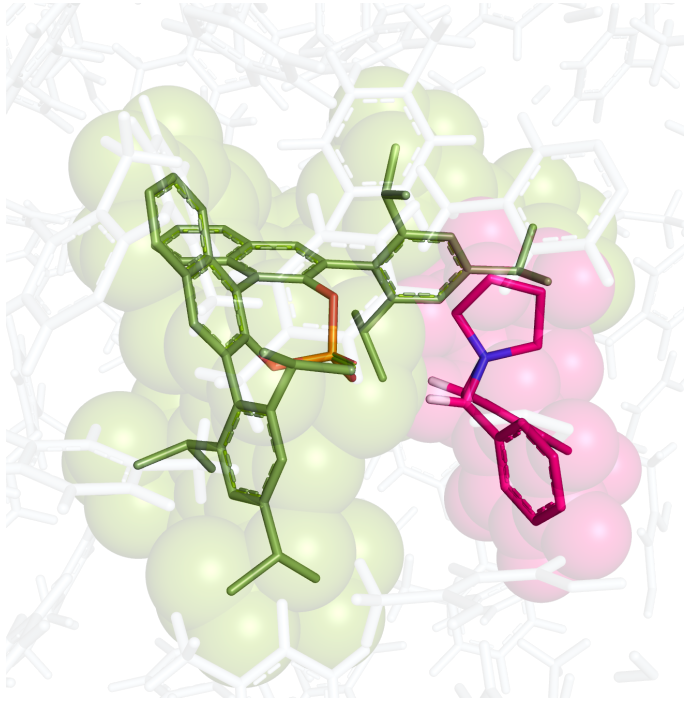


3. Fernanda Duarte: Asymmetric catalysis

- From mechanistic understanding to prediction







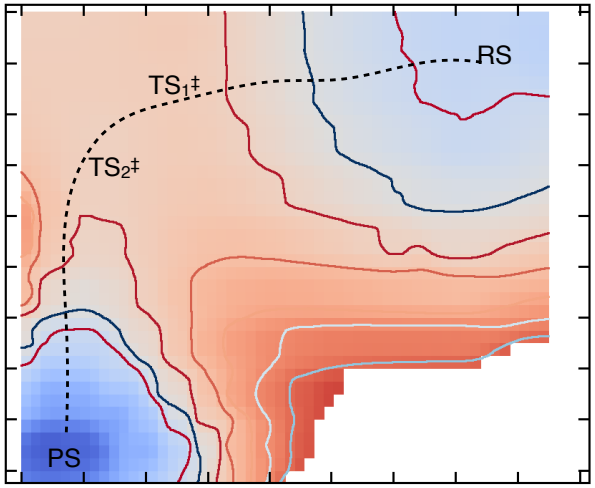
- Most new drugs are marketed as single enantiomers
- Catalyst discovery remains a trial-and-error process

ACS Catalysis **5**, 5702 (2015)
Chem. Soc. Rev. **45**, 6093 (2016)
J. Am. Chem. Soc. ASAP (2017)

3. Fernanda Duarte: Biomimetic catalysis

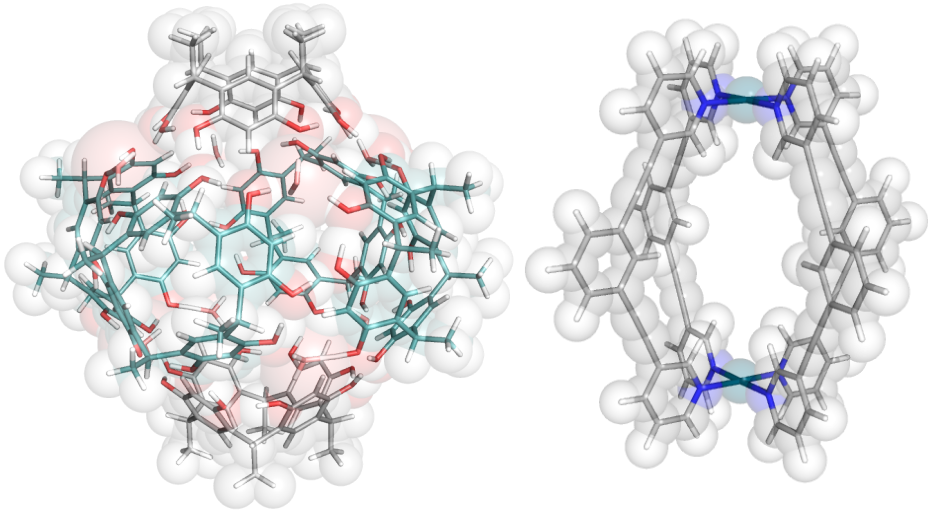
Angew. Chem. Int. Ed. **53**, 8246 (2014)
Angew. Chem. Int. Ed. ASAP (2017)

Reaction Mechanism



Understanding the fundamental chemistry

Supramolecular Chemistry



Exploring Physical / Dynamic properties

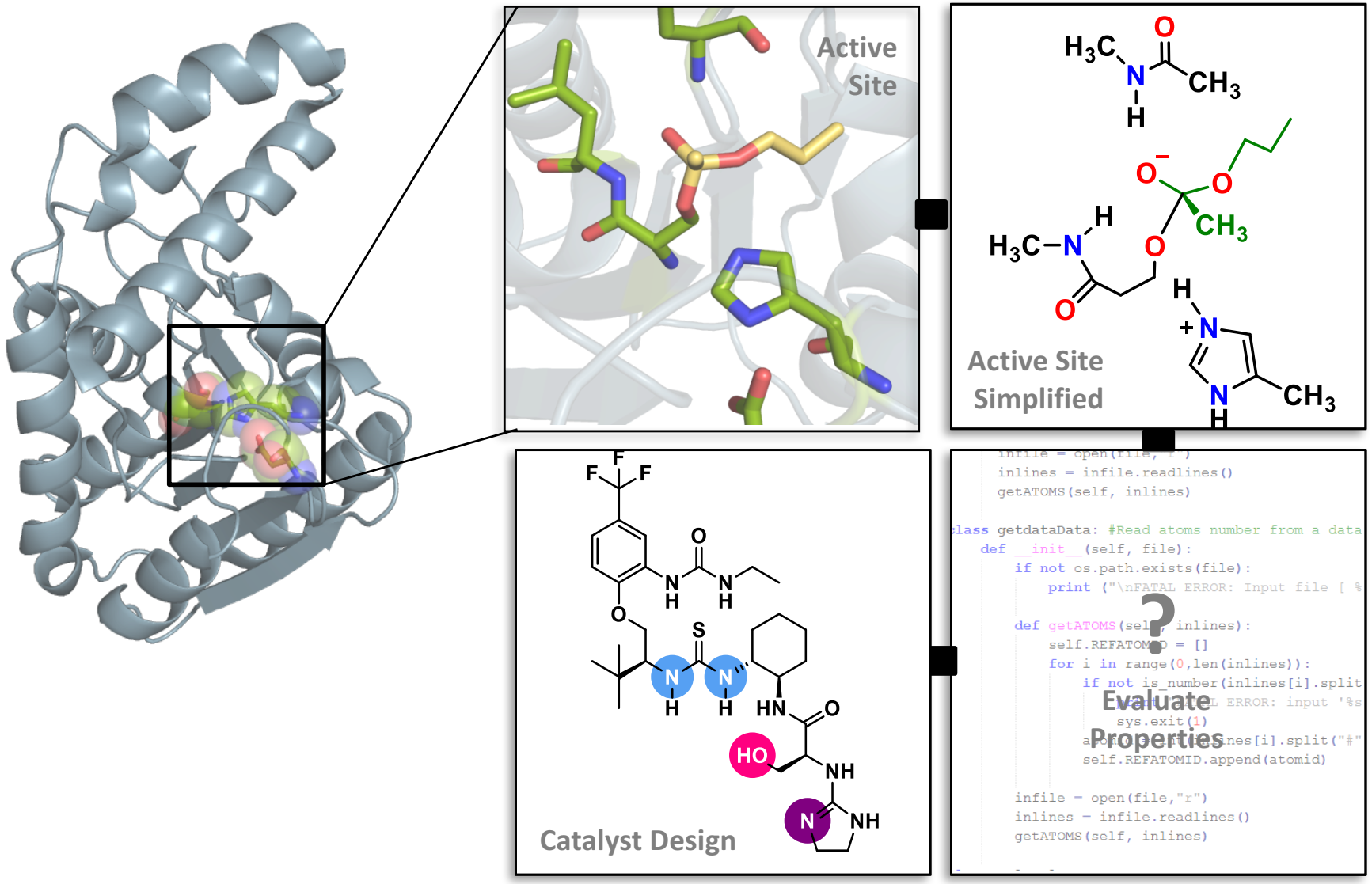
Mechanistic Insights

New Scaffolds

Self-Assembled “Nanozyme”

3. Fernanda Duarte: Biomimetic/enzyme catalysis

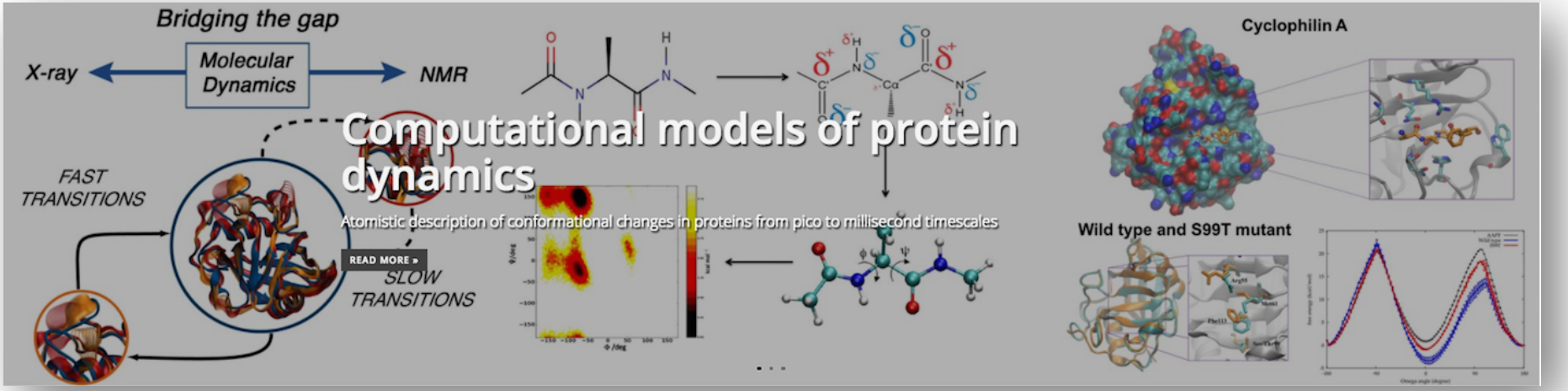
- Using natural scaffolds to introduce catalysis – learning from Nature



4. Julien Michel: Biomolecular systems

- Classical atomistic molecular dynamics

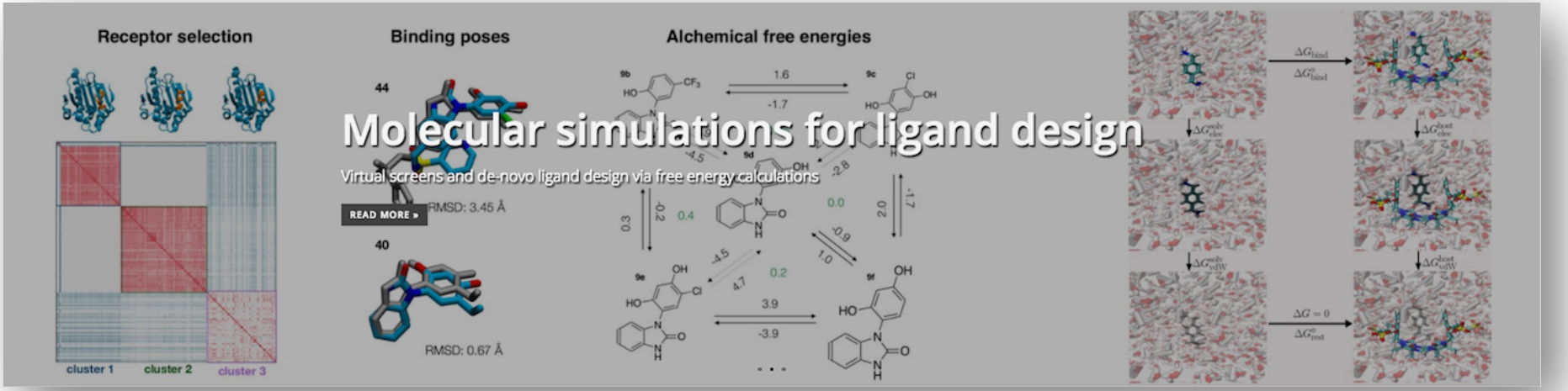
4. Julien Michel: Biomolecular systems



Atomic level description of protein structure and dynamics (picosecond to millisecond) via classical molecular dynamics simulation methods and back-calculation of experimental observables (e.g. NMR spectra)

PLoS Comput. Biol. **11**, e1004282 (2015)

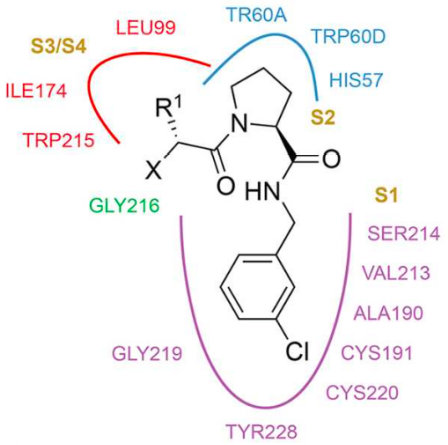
4. Julien Michel: Biomolecular systems

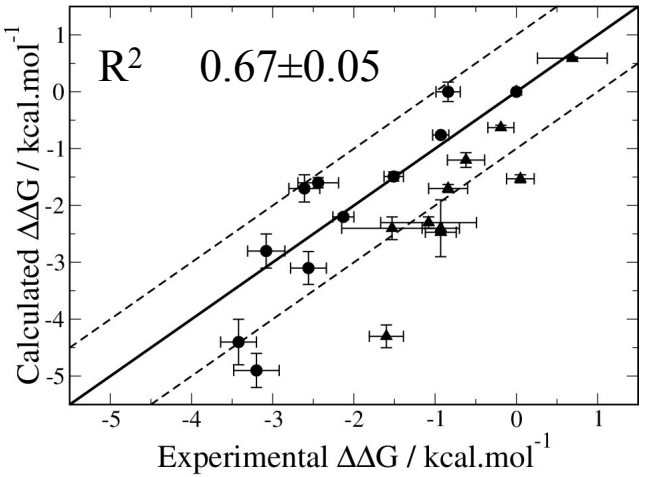


- Molecular simulation algorithms for next-generation computer-aided drug design technologies

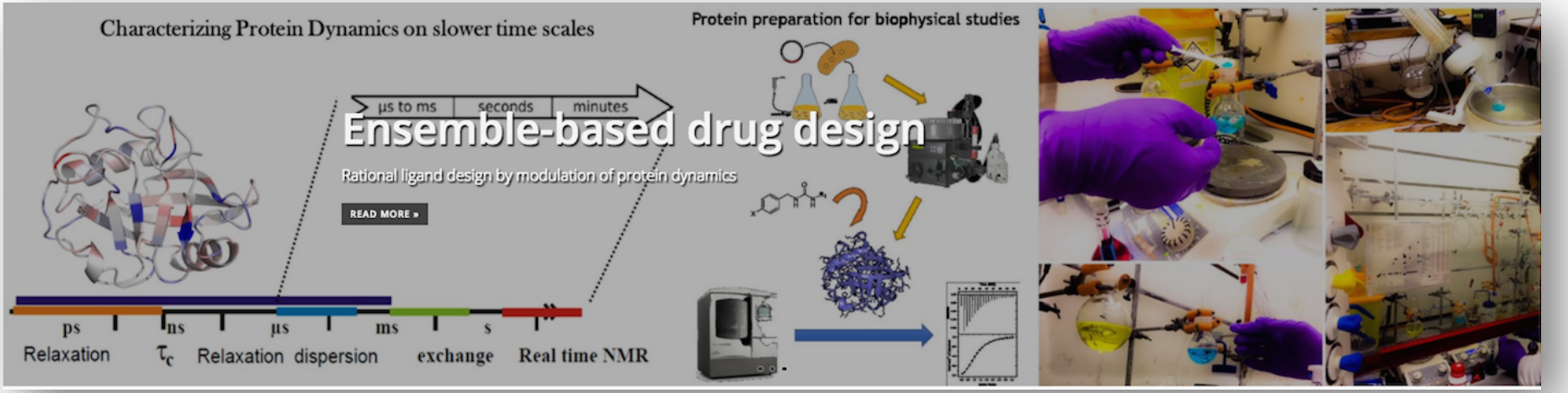
Prediction of binding energies for thrombin ligands by molecular dynamics alchemical free energy calculations

J. Phys. Chem. B **120**, 5340 (2016)



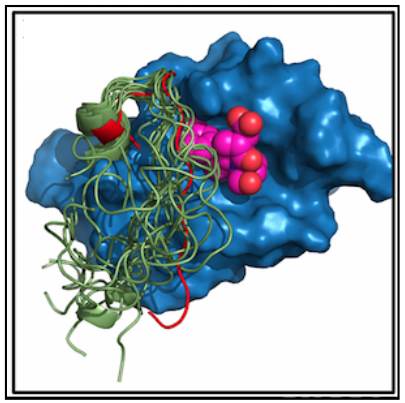


4. Julien Michel: Biomolecular systems

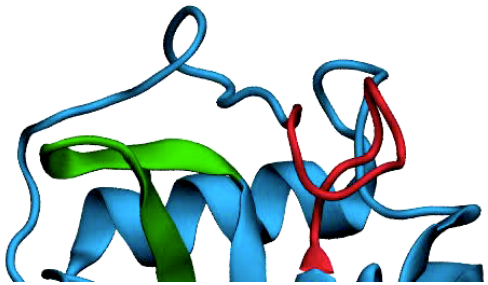


- Combination of molecular modelling, organic synthesis, and biophysical assays methods to deliver improved ligands for challenging drug targets via modulation of protein dynamics

MDM2 lid dynamics (cancer)



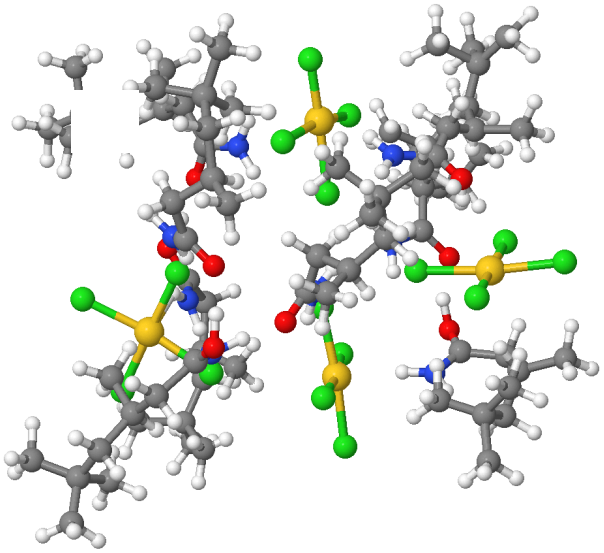
Cyclophilins loops dynamics (viral infections, neurodegenerative diseases)

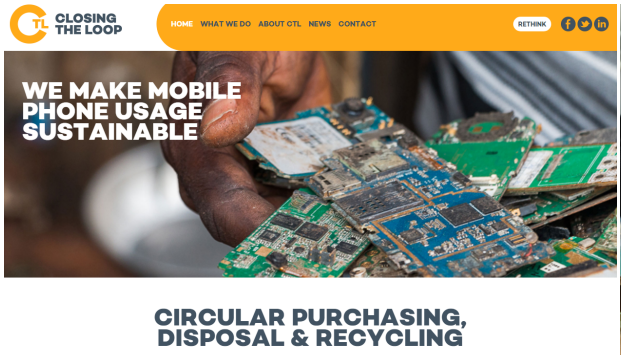


4. Carole Morrison: Molecular liquids

- **Ab-initio and classical molecular dynamics**
  Jason Love, Mary Healy, Peter Tasker, Innis Carson, Rebecca Nicolson, Euan Doidge, and Jamie Hunter

- Urban mining – recovering wealth from waste electronics
- Designing and understanding sustainable processes to recover, e.g., gold (selectively!) from printed circuit boards





Angew. Chem. Int. Ed. **55** 12436 (2016)
Infinite Magazine (UoE/ERI) Issue 14, October 2015

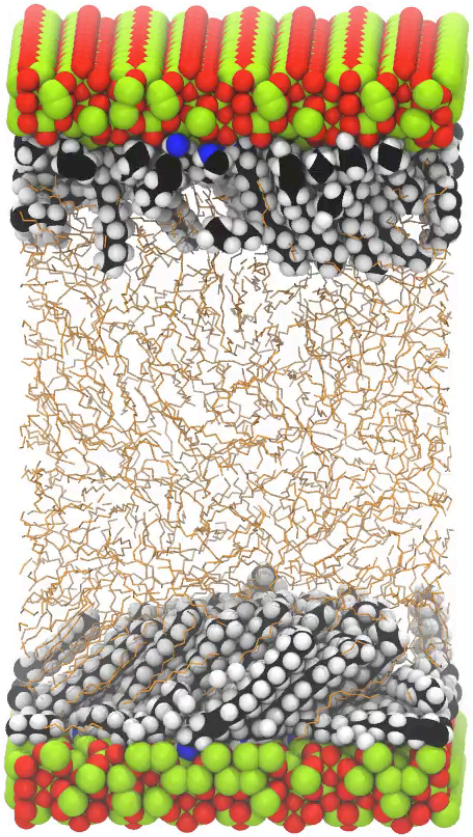
4. Philip Camp: Molecular liquids

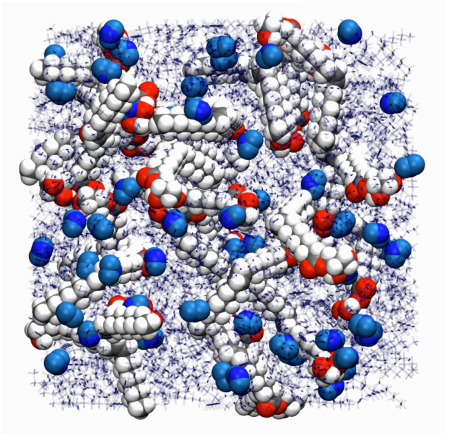
- **Classical molecular dynamics**

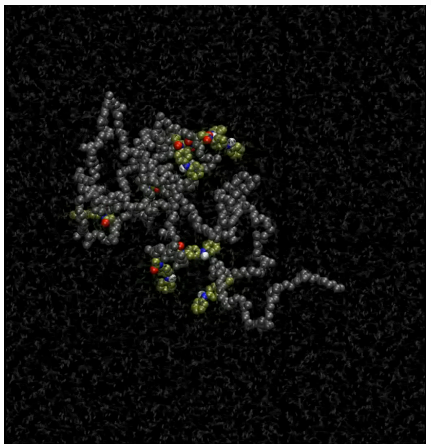
4. Philip Camp: Molecular liquids

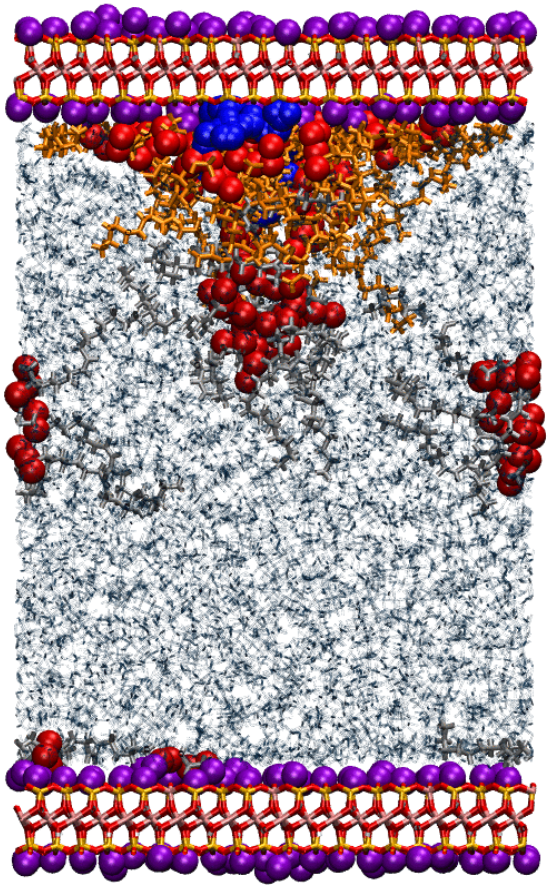
- Self-assembly, adsorption, and friction in lubricants
  Rui Apóstolo and Georgia Tsagkaropoulou

Langmuir **30**, 186 (2014)
J. Phys. Chem. B **55** 12436 (2015)
Phys. Chem. Chem. Phys. **17**, 5248 (2015)
Langmuir **32**, 7707 (2016)





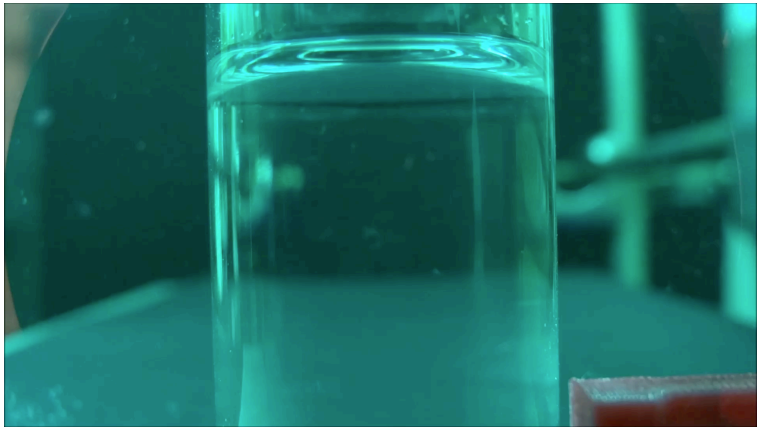




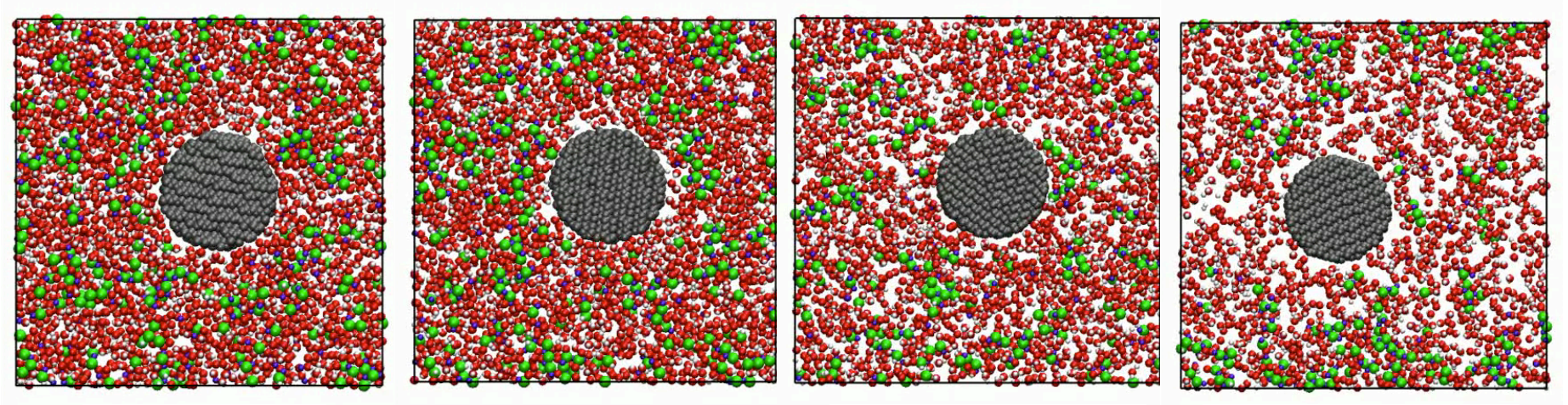
4. Philip Camp: Molecular liquids

- Non-photochemical laser-induced nucleation
  Andrew Alexander and Julien Sindt

J. Phys. Chem. B **118**, 9404 (2014)



- Nanoparticle heating in aqueous salt solutions

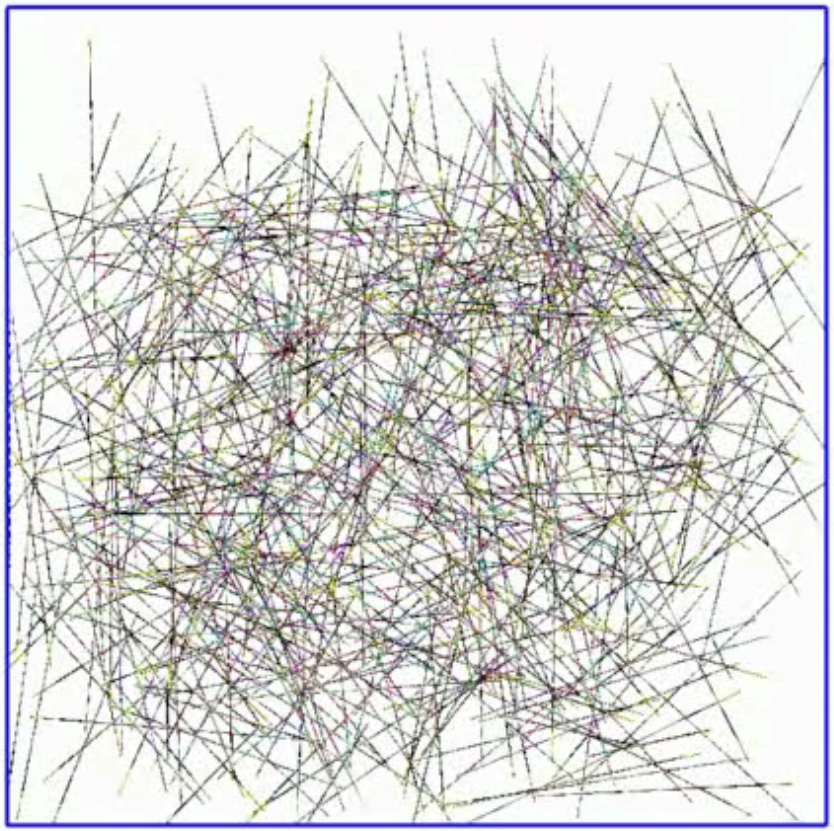


equilibrium $t = 0.0{-}0.1$ ns $t = 0.9{-}1.0$ ns $t = 2.3{-}2.4$ ns

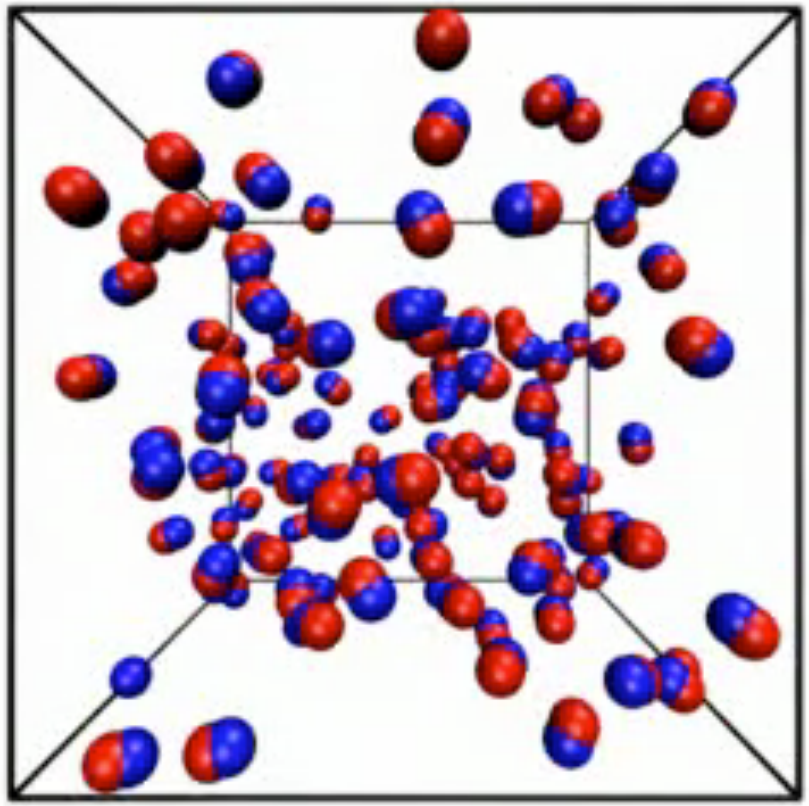
5. Philip Camp: Soft matter

- **Coarse-grained dynamics**
  Fabio Nudelman and Julien Sindt

Collagen fibril formation
Aggregation kinetics



Magnetic colloids
AC field-induced hyperthermia



Phys. Rev. E **93**, 063117 (2016)

MD Simulations in the School of Chemistry

1. **Few-atom quantum molecular dynamics**
   Adam Kirrander

2. **Ab-initio and Car-Parrinello molecular dynamics**
   Carole Morrison

3. **Quantum mechanics/molecular mechanics**
   Fernanda Duarte

4. **Classical atomistic molecular dynamics**
   Philip Camp, Julien Michel, Carole Morrison

5. **Coarse-grained dynamics**
   Philip Camp