- **Teokem: the science we do with LUNARC**
  - **Jan Forsman**
  - **Mikael Lund**
  - **Petter Persson**
  - **Ulf Ryde**
  - **Marie Skepö**
  - **Martin Trulsson**
  - **Valera Veryazov**

SWOT analysis of Teokem-LUNARC relations

S

- Long history together with LUNARC
- Joint projects in the past and the present
- (sometime) intensive use

O

- Education for developers e.g. parallel/GPU coding
- Diversity in hardware (cores/RAM/disk)
- Compilers, profilers, debuggers

W

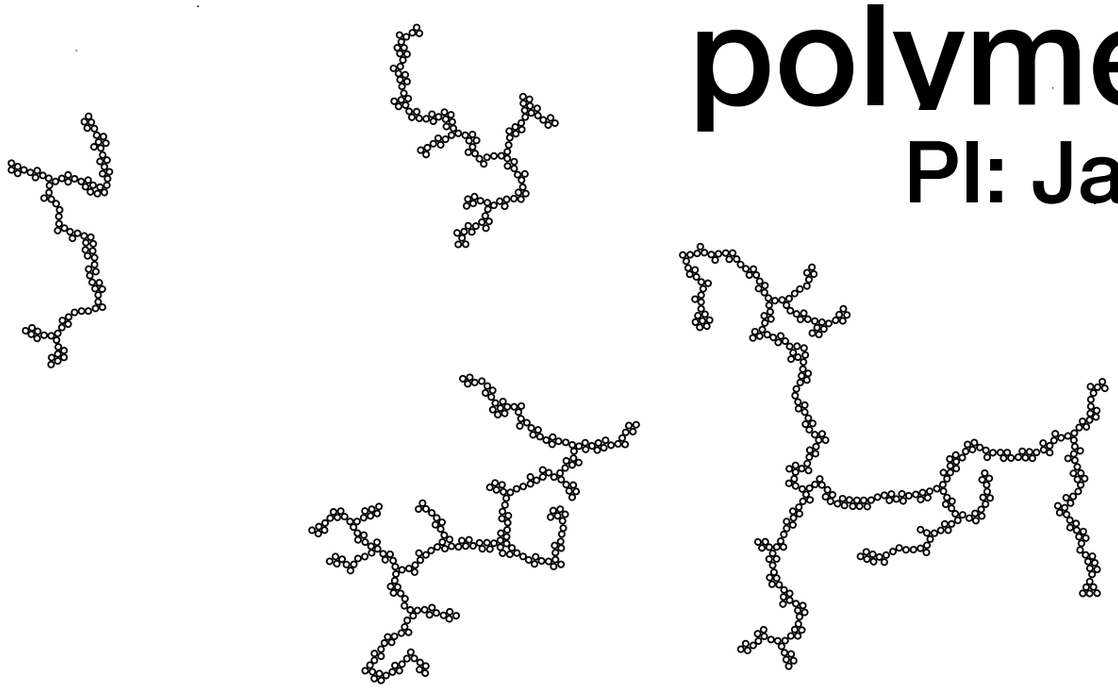
- Software needs do not match hardware (e.g. RAM per core)
- Rigid allocation system
- Optimization (GPU, parallel) requires huge efforts and support

T

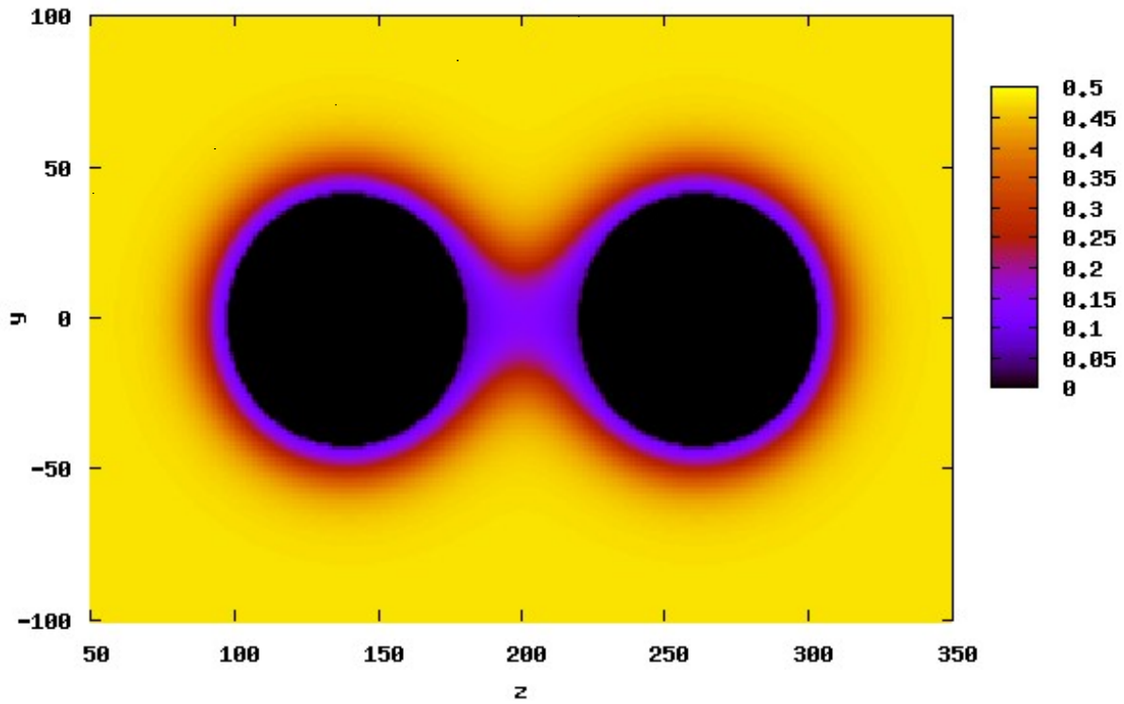
- Moving back to local clusters
- Migration to other supercomputers
- Use of resources in inefficient way

Coulomb fluids and polymer solutions

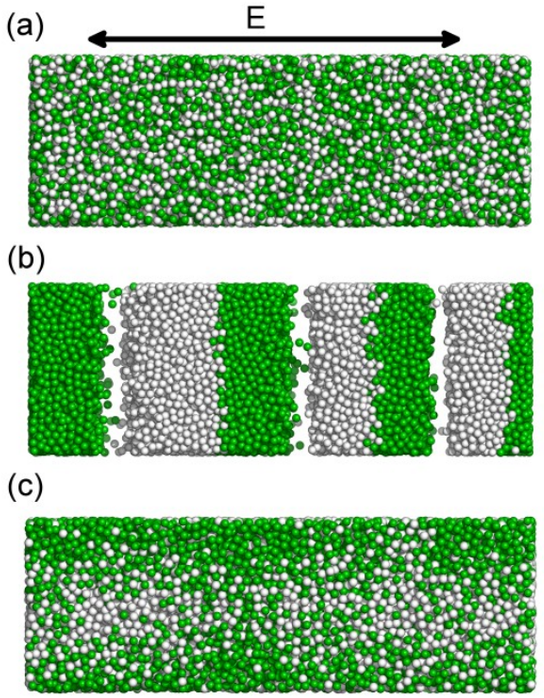
PI: Jan Forsman

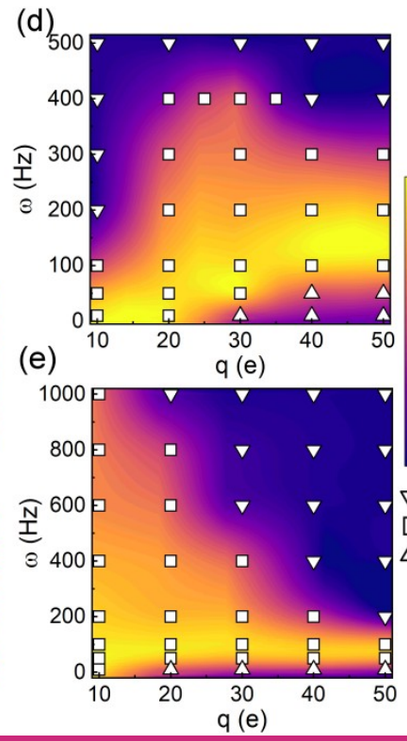


anisotropic structures from isotropic interactions



polymer-induced particle interactions



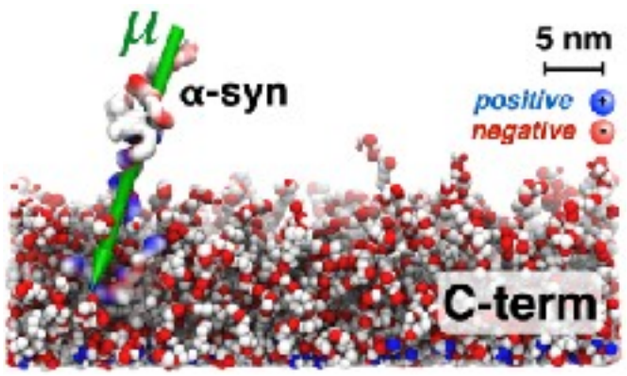


Field-induced jamming

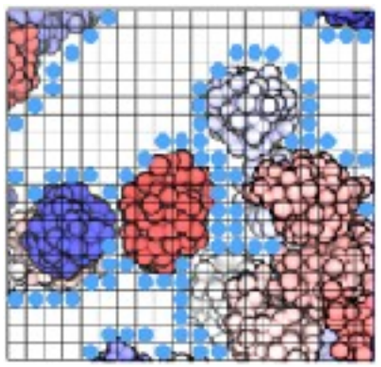
Tools at lunarc:

- **Fortran compilers**
- **Slurm (obviously)**
- **Cpu:s (mainly) and storage**

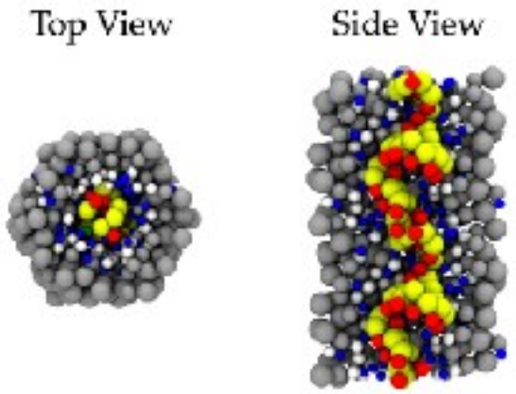
Biomolecular Interactions and Multiscale Simulations



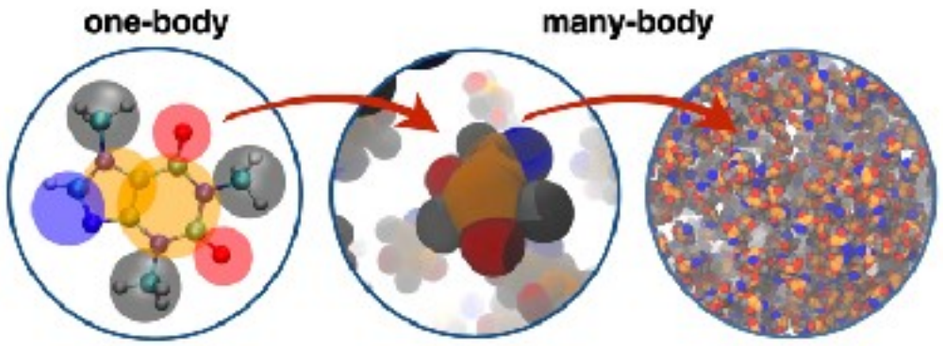
Peptide-surface interactions
(With Sara Linse, Emma Sparr)



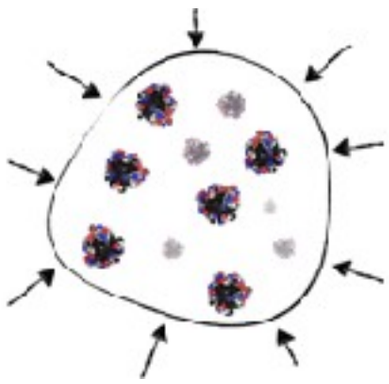
Scattering calculation of proteins and inclusion of solvation layers
(LINXS and w. Jan Skov Pedersen)



pH dependent lipid encapsulation of mRNA for drug delivery (with Astra Zeneca).
This very new technology is used in e.g. the Pfizer and Moderna COVID-19 vaccines.



Multiscale simulations of caffeine and small biomolecules in aqueous salt solutions



Osmotic stress calculations on concentrated protein solutions

Tools and resources:

- MD software: Gromacs, OpenMM
- Own software: "Faunus" (c++17, MPI, OpenMP). https://github.com/mlund/faunus
- GCC and Intel compilers; cmake
- Lunarc desktop
- Anaconda; Jupyter Notebooks
- Storage; CPU; GPU

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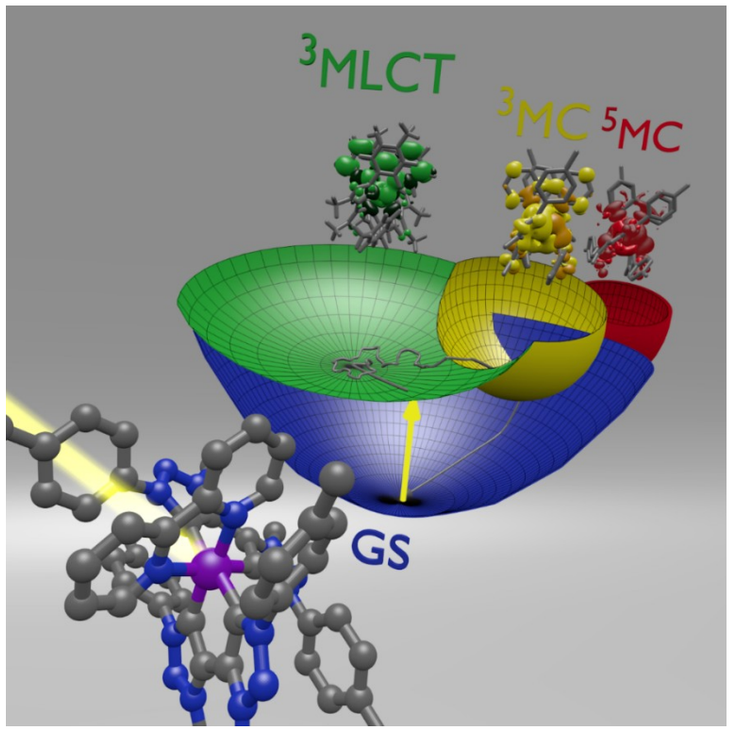
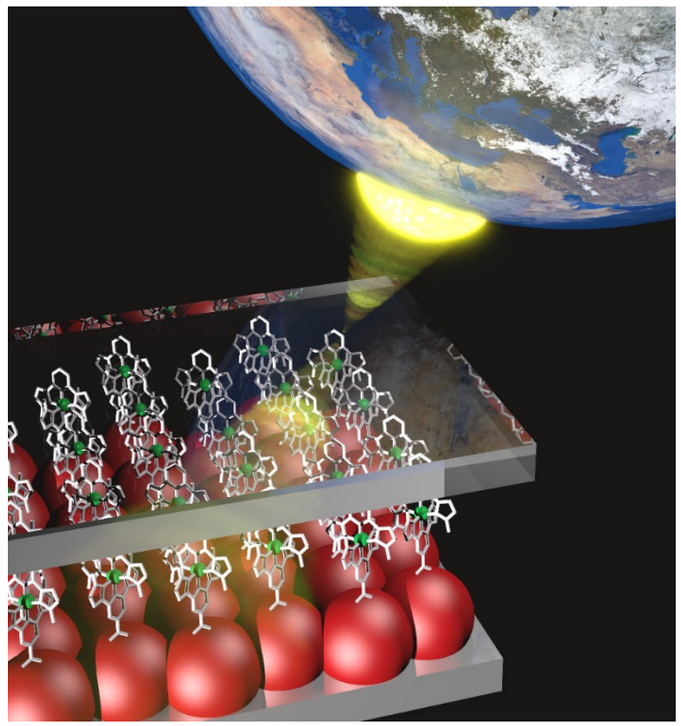
Solar Energy Conversion Calculations

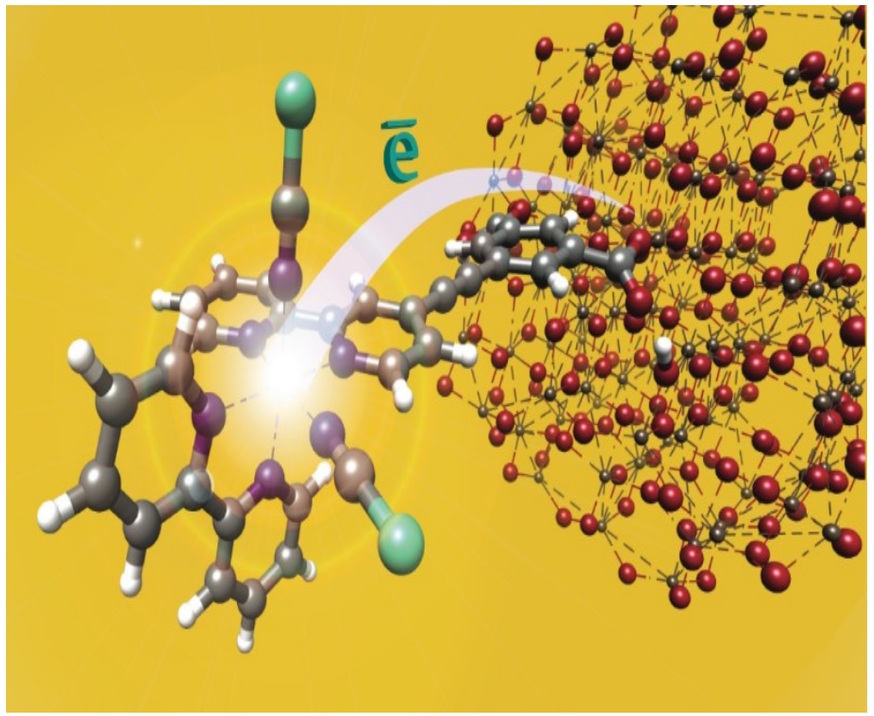
PI: Petter Persson



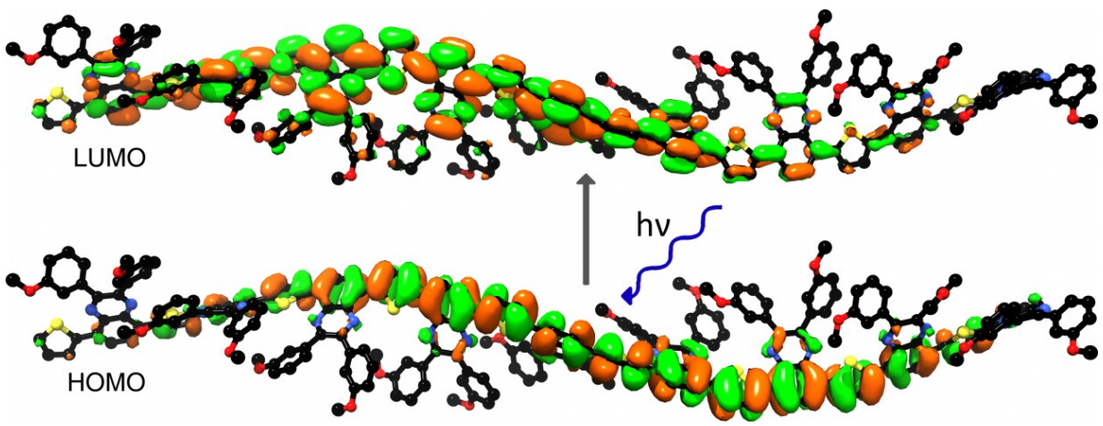
Molecular Photocatalysis



Quantum Photoelectrochemistry



Surface Functionalization of Nanostructured Semiconductors



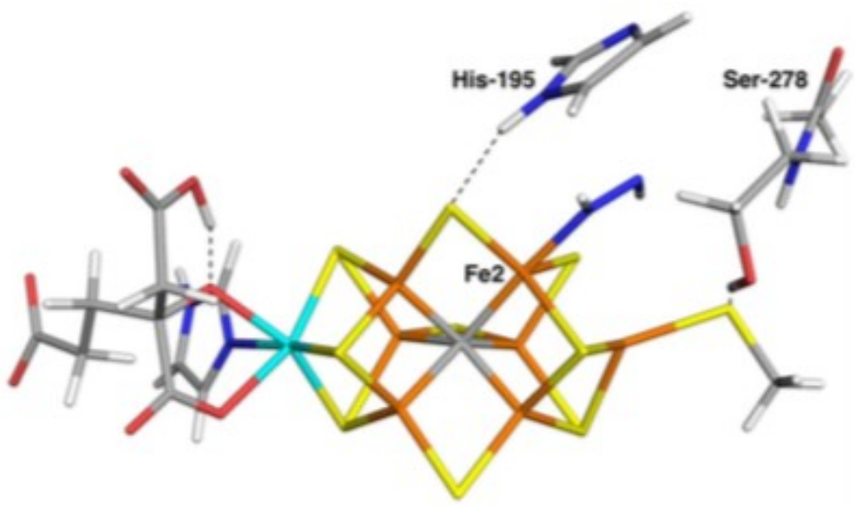
Molecular Electronics and Organic Photovoltaics (OPV)

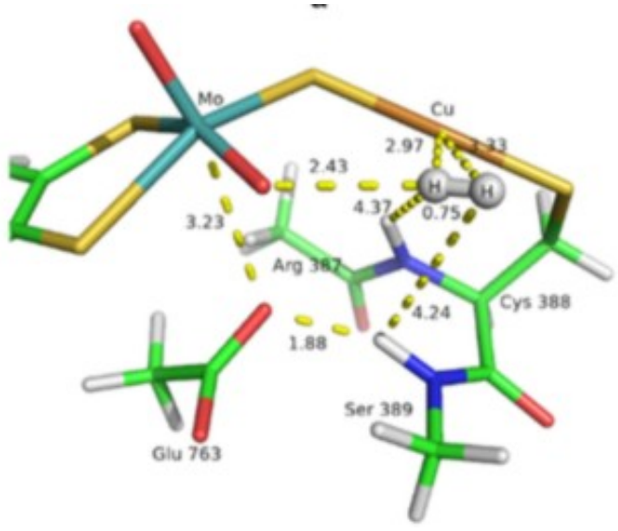
LUNARC tools

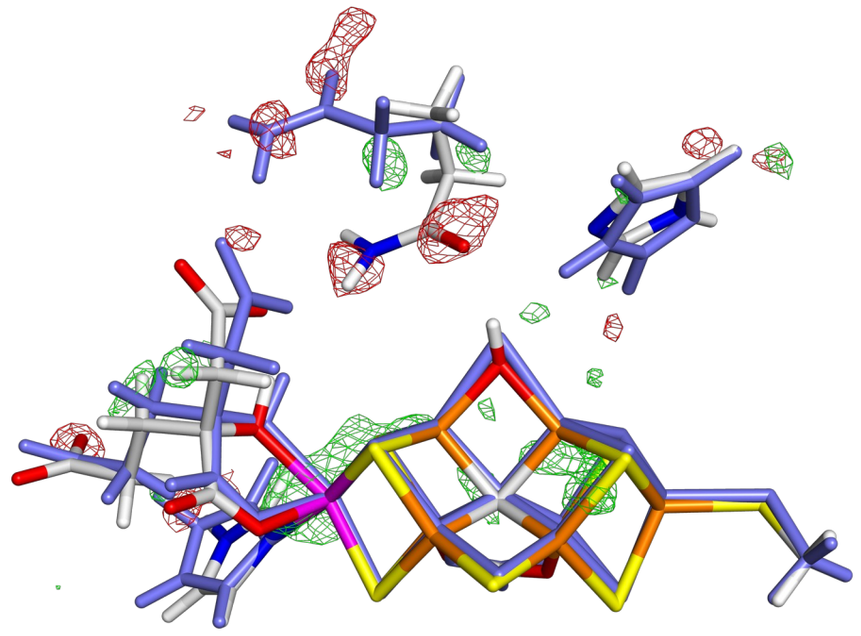
- **Quantum Chemistry programs: Gaussian, Orca, etc**
- **Python**
- **CPU:s and storage**

Biological Systems

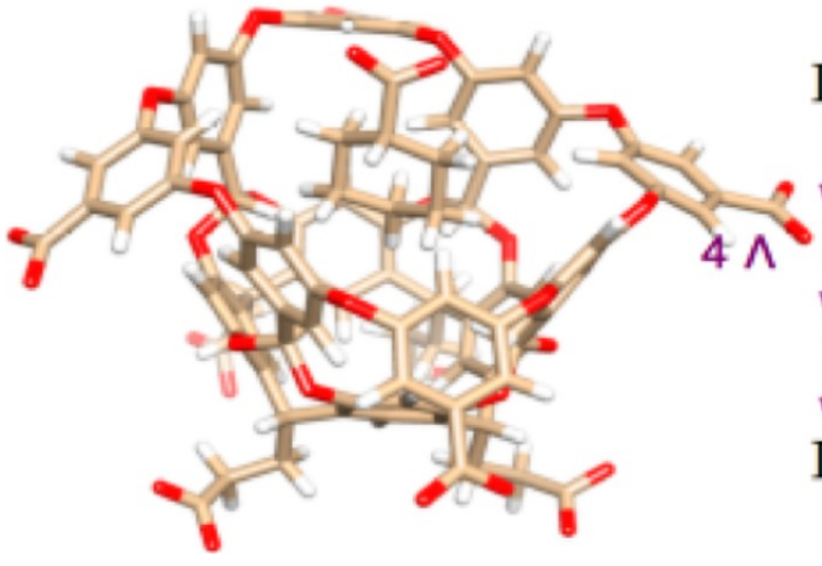
PI: Prof. Ulf Ryde

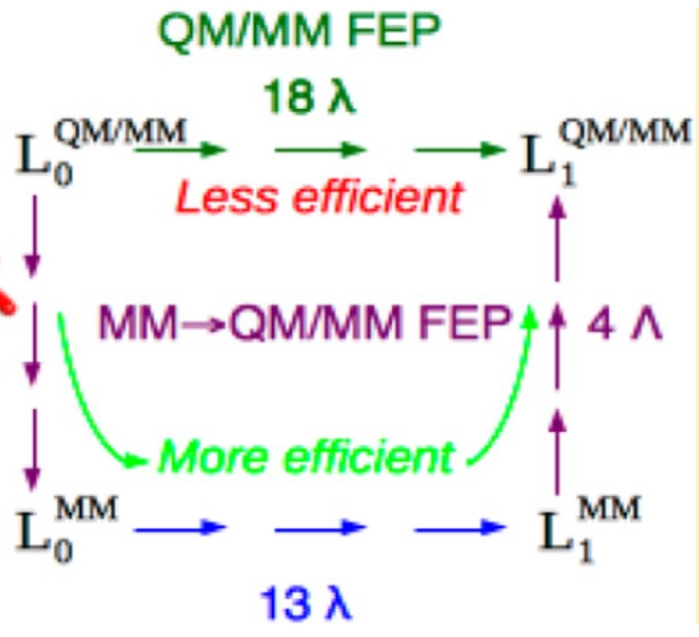






Function and mechanisms of metalloproteins
Nitrogenase, hydrogenase, methane monooxygenase, etc.





Ligand binding – drug development
Improve accuracy by QM calculations

Improving X-ray and neutron crystallography
Using QM and MD calculations

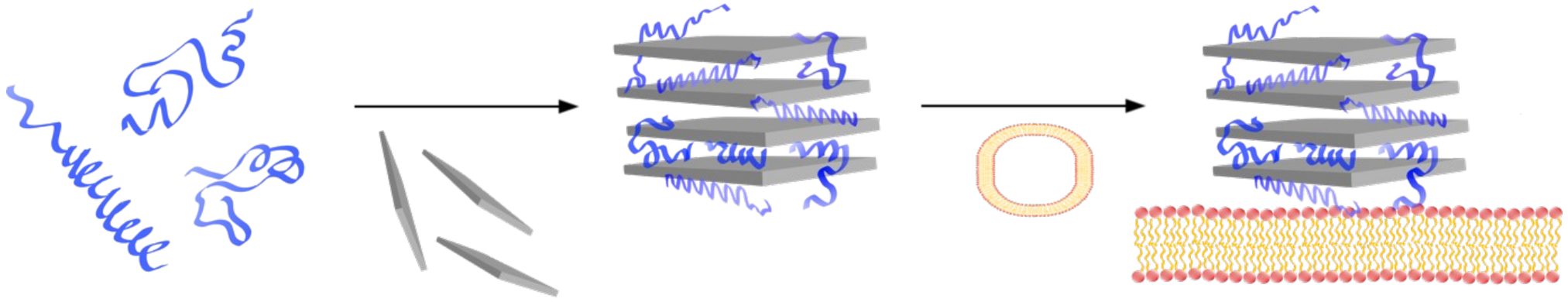
Methods:

- QM/MM
- Molecular dynamics
- Free-energy perturbations
- CASPT2 / DMRG-PT2
- Quantum refinement

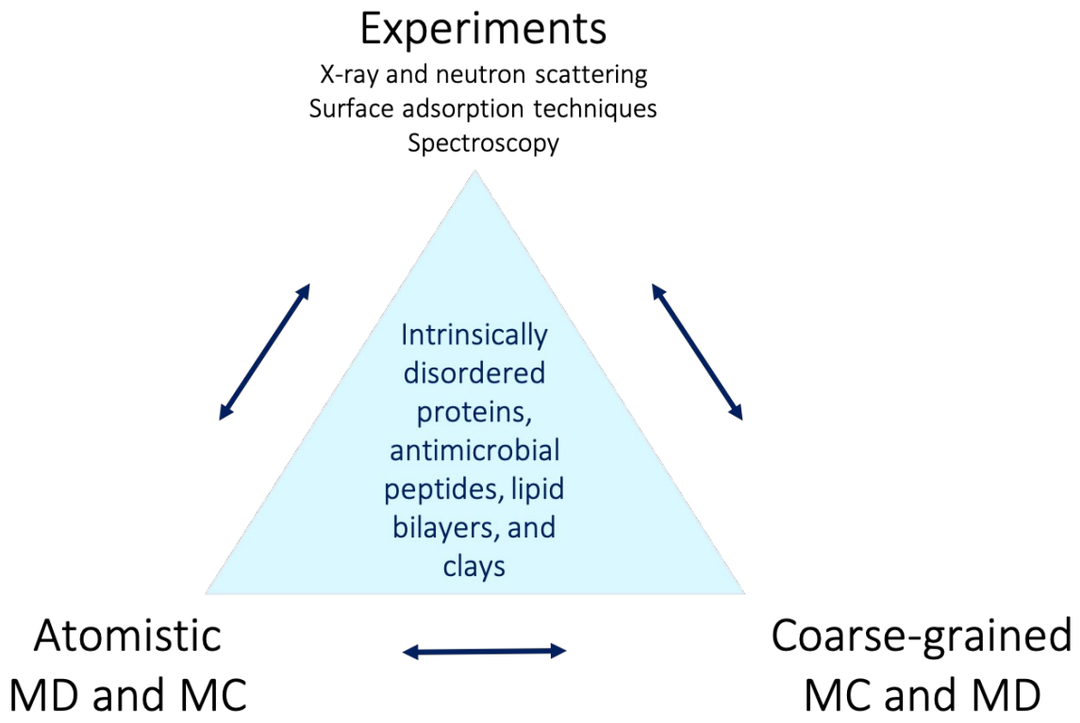
Biological and Colloidal Systems

Next Generation Structural Biology

PI: Marie Skepö



Bulk solution → Interaction with Surfaces
Single Molecule → Crowded Solutions

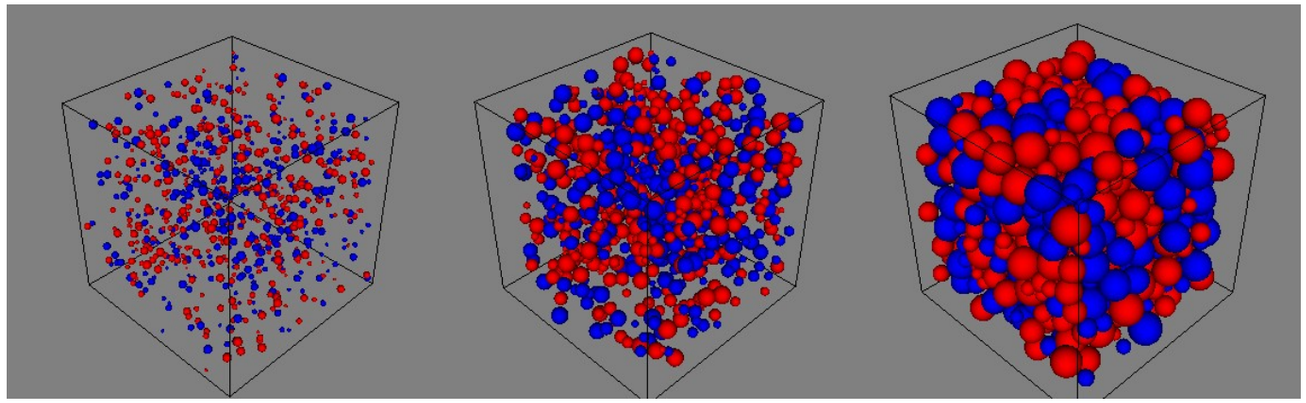


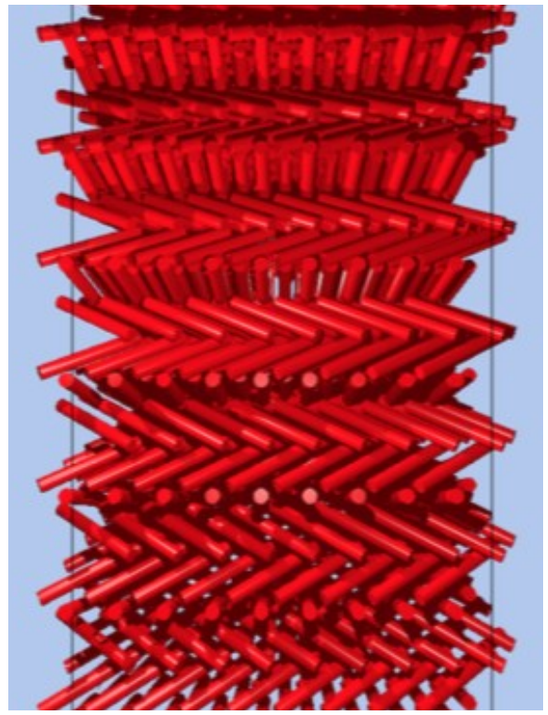
LUNARC tools

- **Gromacs**
- **Python**
- **CPU:s/GPU:s and storage**

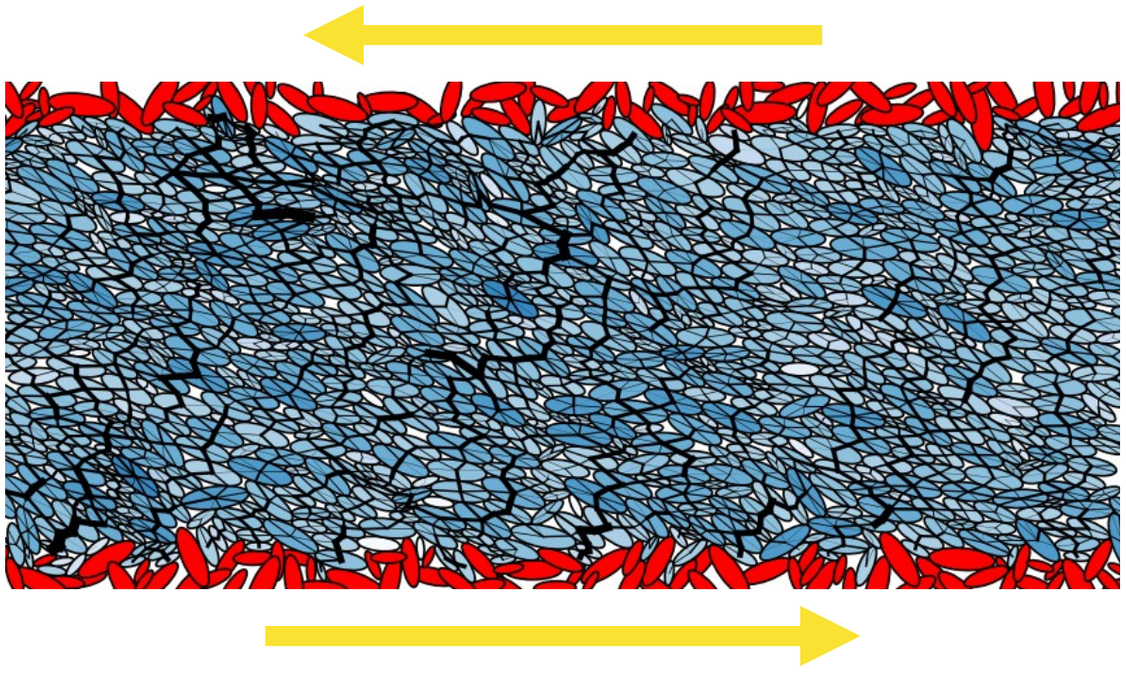
Granular and suspension flows lab

PI: Docent Martin Trulsson





Drying of polymer films/gels - Brownian dynamics simulations



Phase diagram of crystalline nanocellulosa – Monte Carlo simulations and brute force calculations

Rheology of granular and dense suspensions - DEM modelling

Tools at LUNARC:

- GCC/ICC
- Python numpy/scipy/matplotlib
- Slurm (obviously)
- CPU:s and storage

Electronic structure: from atoms and molecules to crystals
PI: Valera Veryazov

OpenMolcas developers

IT support

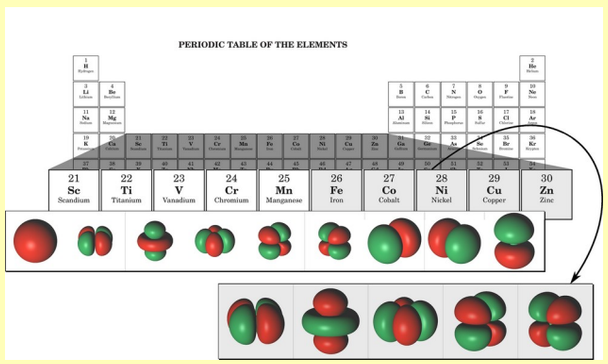
→ OpenMolcas →

Stable releases for Molcas users

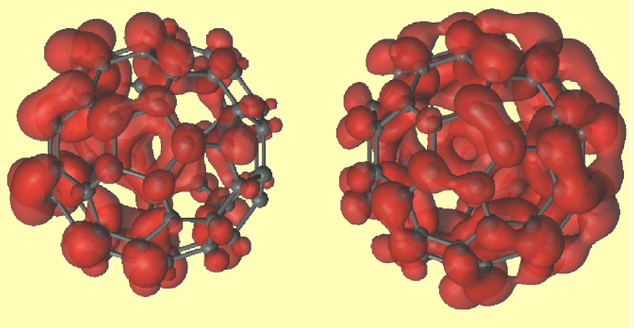
Performance efficient
Parallel
Use linear algebra libraries

High RAM demand
Low efficiency at modern HW
Sensitive to MPI variants

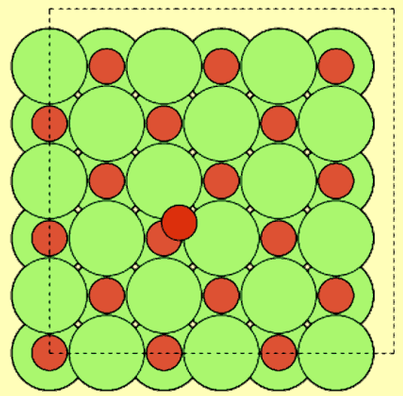
New atomic basis set ANO-R



Symmetry of electronic structure of $(C_{60})_2$



Embedded cluster:
O diffusion on MgO surface



Interaction with LUNARC: use of resources, development, optimization