EPSRC
Pioneering research and skills

ARCHIE-WeSt

Academic and Research Computer Hosting Industry and Enterprise in the West of Scotland

www.archie-west.ac.uk

Karina Kubiak-Ossowska

University of Strathclyde Glasgow
University of Glasgow
GCU Glasgow Caledonian University
University of Stirling
UWS University of the West of Scotland

ARCHE-WeSt and me

HPC User Support officer:

- Project and account management
- Linux and HPC training
- User Support
- Advanced Molecular Dynamics training and support

  Training delivered:

  - locally (for Consortia Users)
  - Nationally (with EPCC)
  - Internationally (BIT workshops abroad)
- Own research activity

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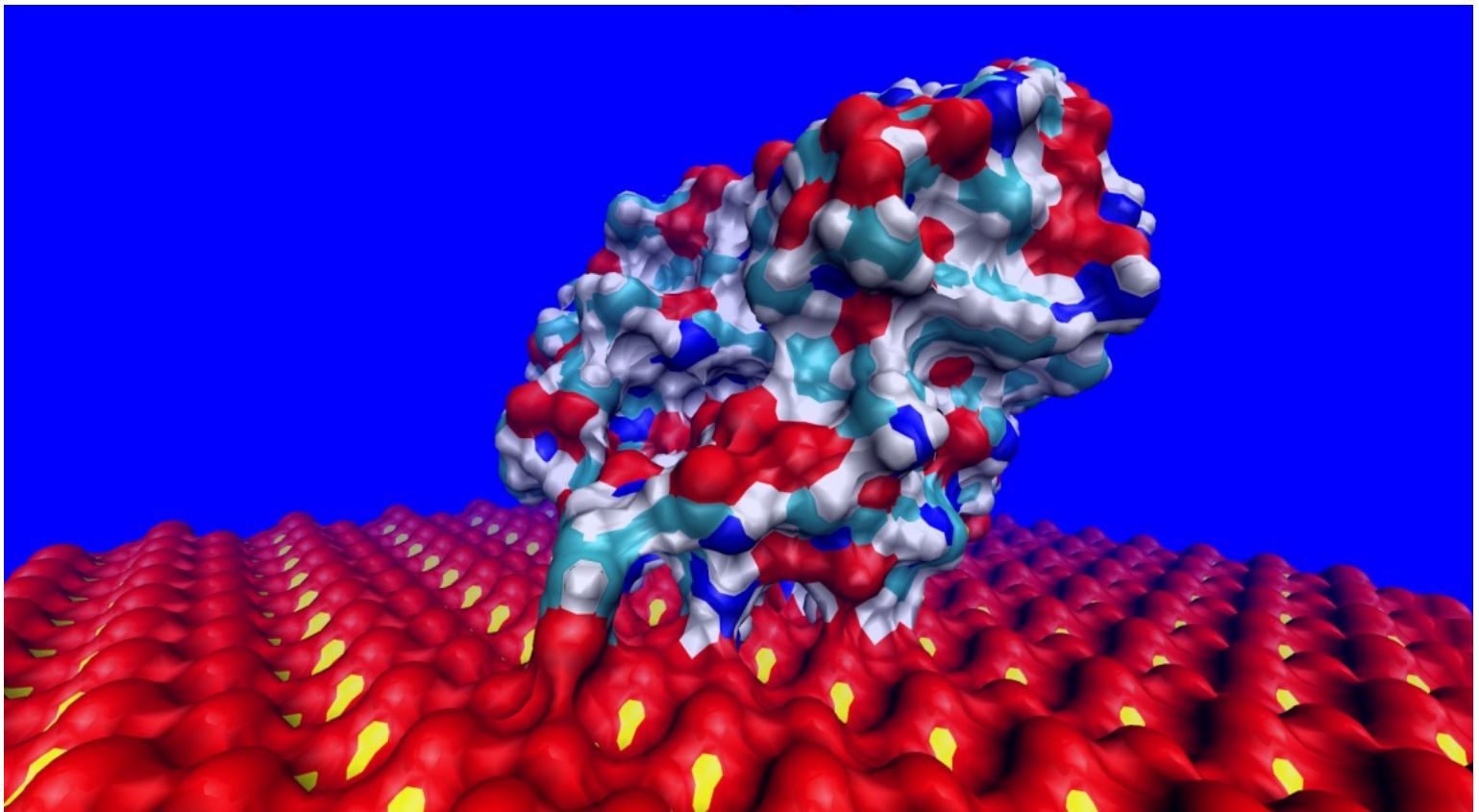
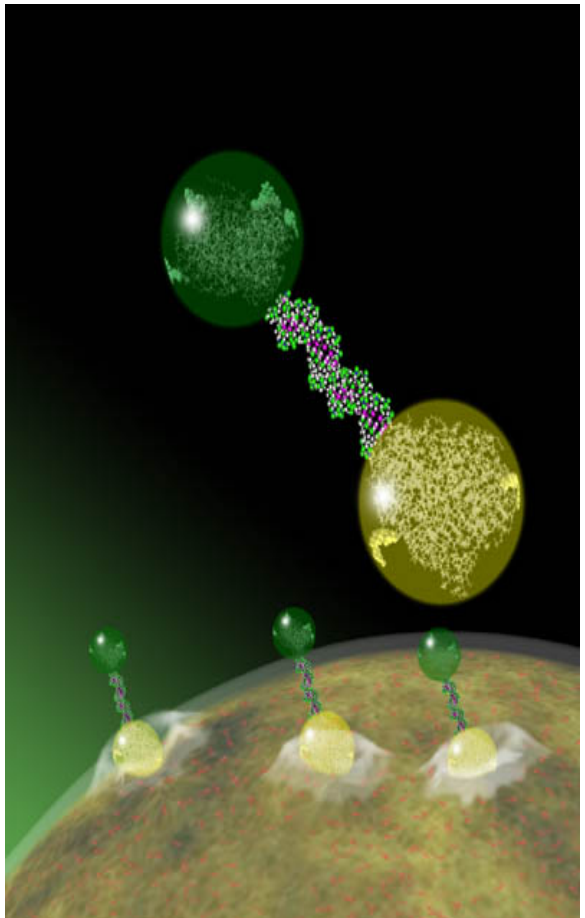
Engineering

Modelling Protein Interactions with Nanoparticles and Material Surfaces



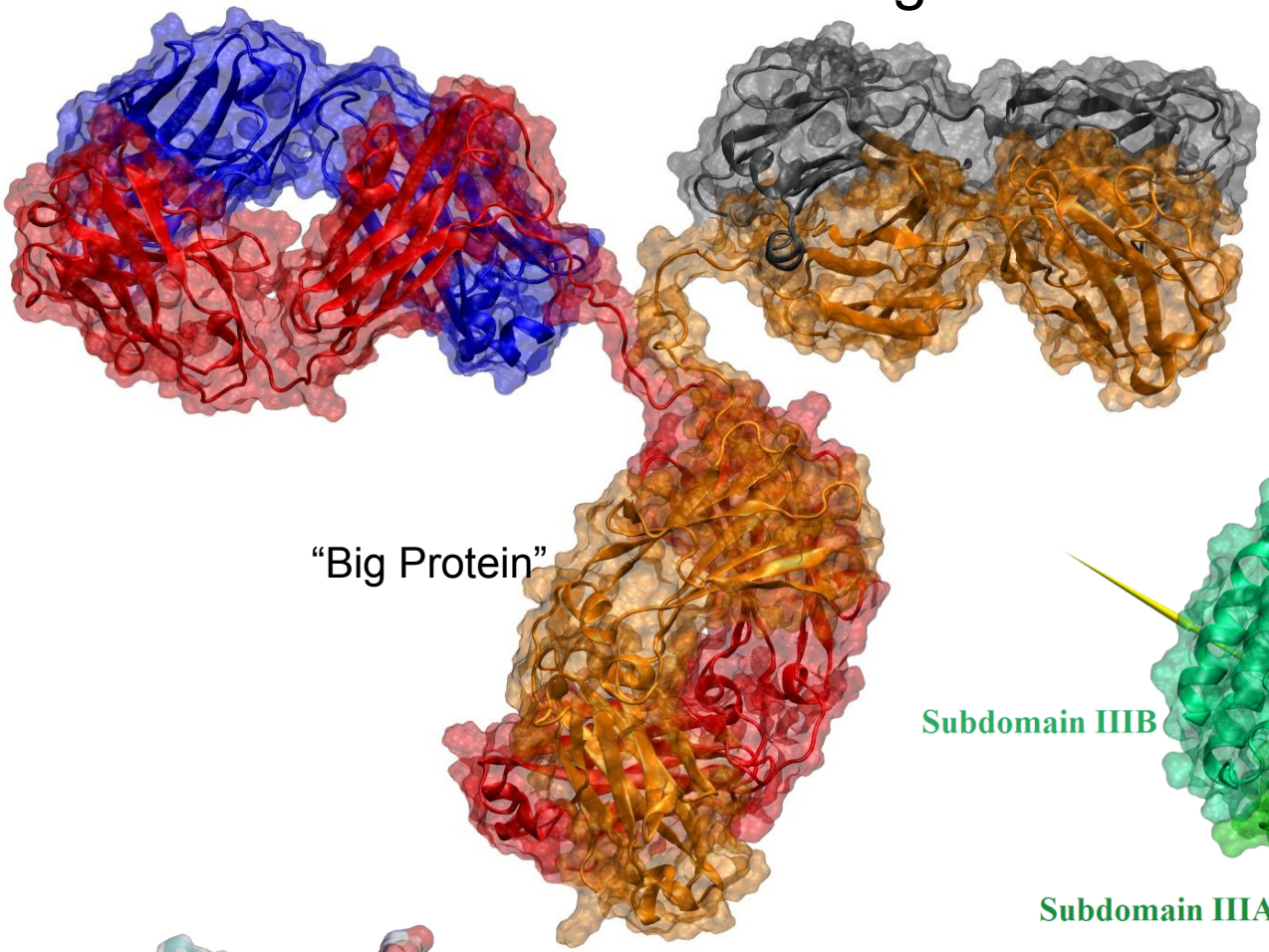
Motivation

The interactions between proteins and nanoparticles/solid surfaces are essential for a number of applications (biomaterials, medical implants, drug delivery systems, nanomedicine, diagnosis, food storage, nanofood etc)

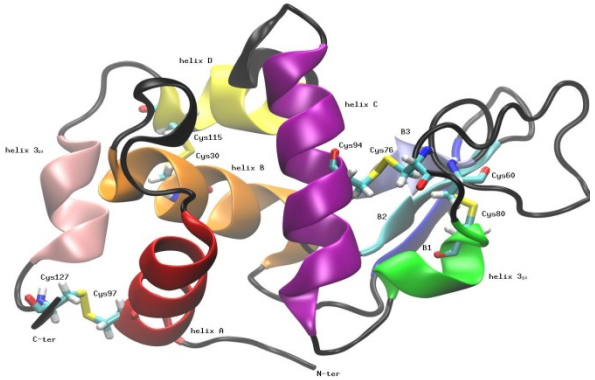


Model proteins

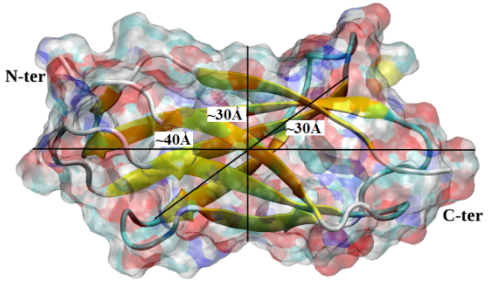
Once we understand how things work we can manipulate them



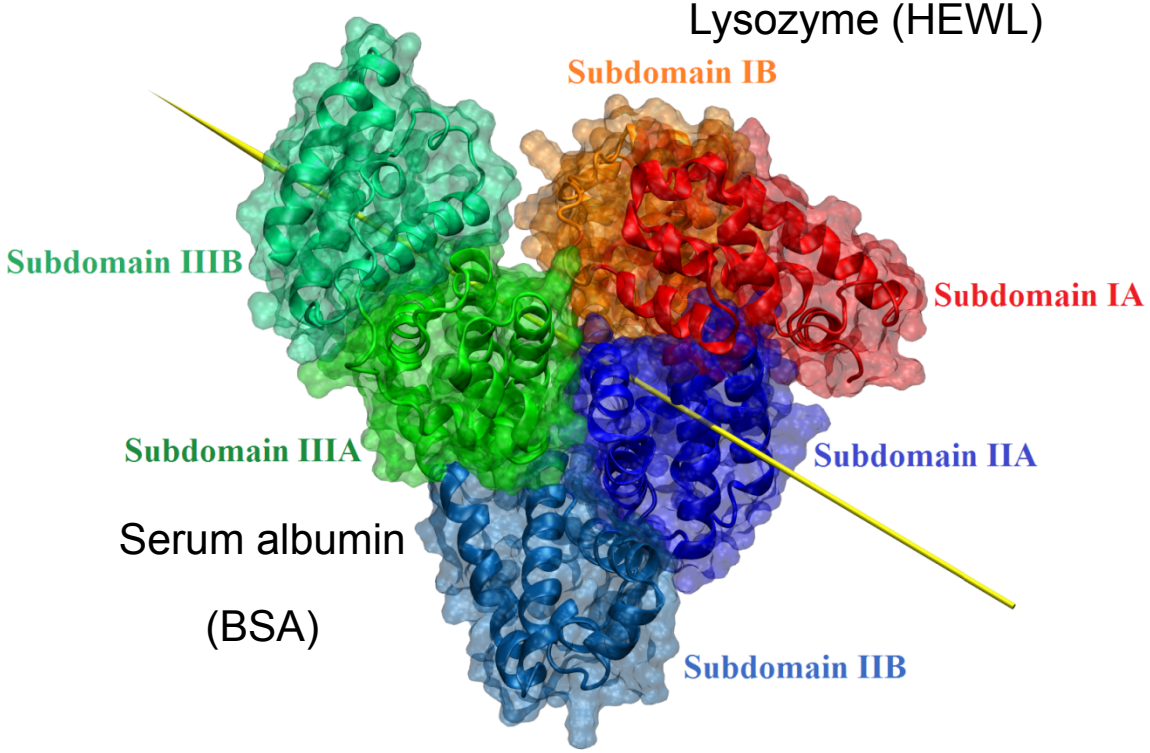
"Big Protein"



Lysozyme (HEWL)



FN^{III}9 (module)



Serum albumin

(BSA)

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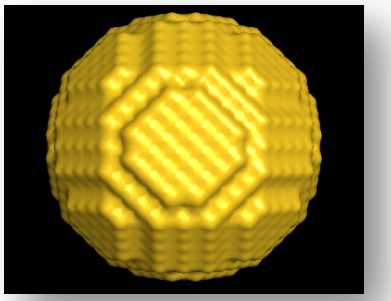
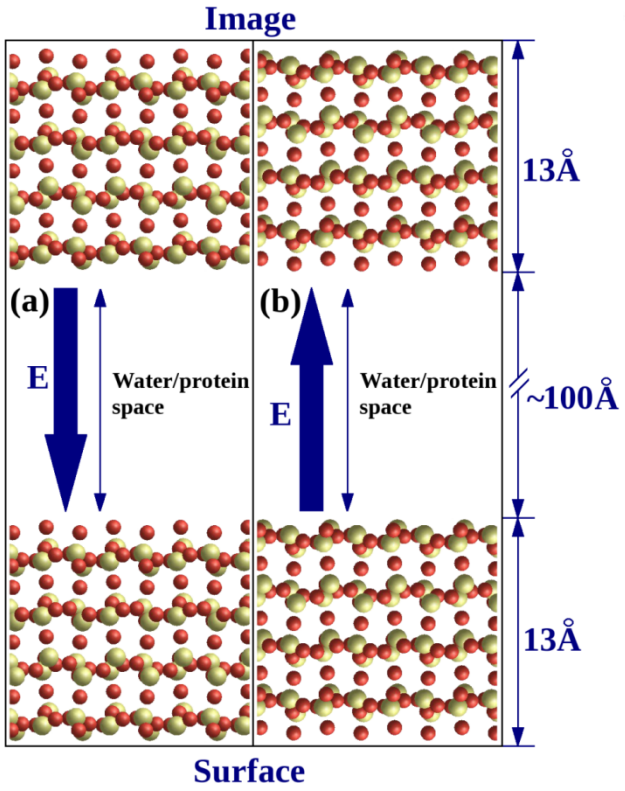
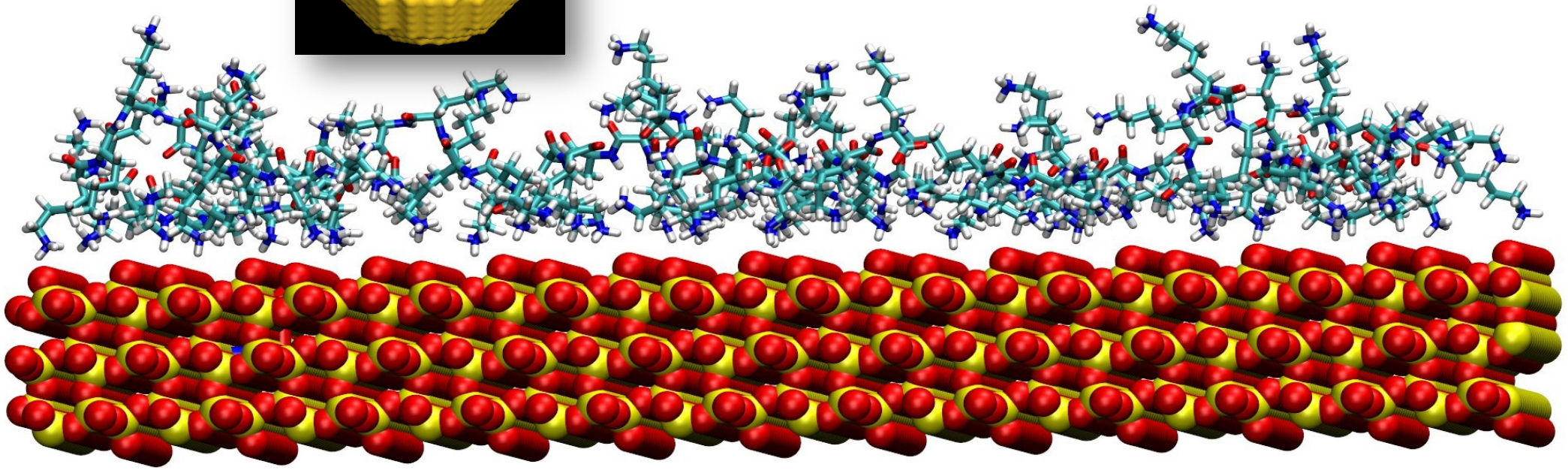
Model surfaces

- ✓Mica
- ✓Silica
- ✓Gold
- ✓Functionalized silica
- ✓Gold Nanoparticles

ø 5nm







Model systems

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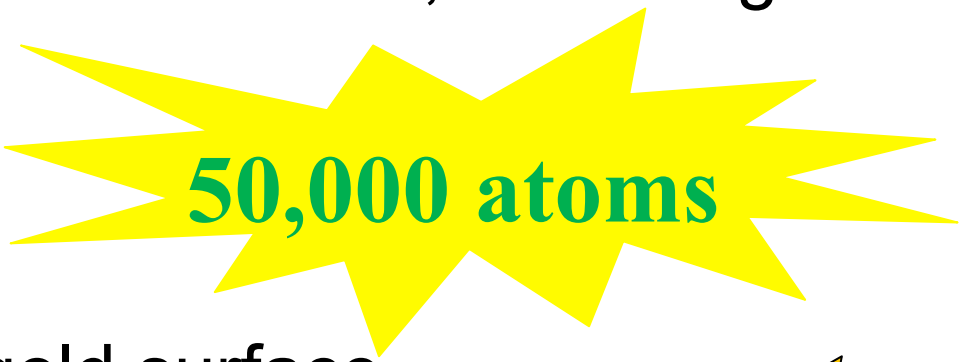
- ✓Lysozyme and FN module on mica, silica or gold surface
  - protein (2k atoms)
  - surface (8k atoms)
  - water (40k atoms)



- ✓ Albumin on silica or gold surface
  - protein (9k atoms)
  - surface (14k atoms)
  - Water (220k atoms)

- ✓"Big Protein"on surface or with Au NPs
  - Protein (20k atoms)
  - Surface (17k atoms)
  - Water (400k – 600k atoms)

- ✓Functionalized silica or NPs– system has to be even bigger

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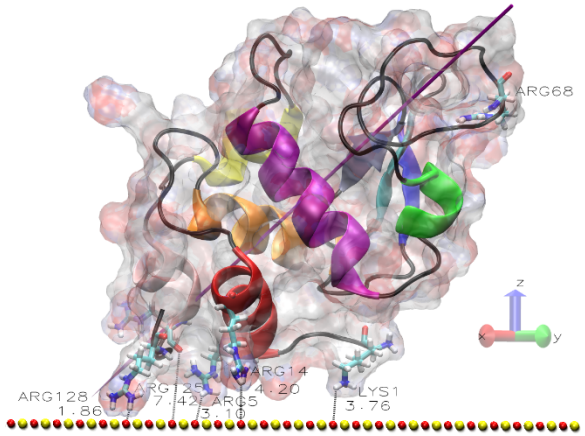
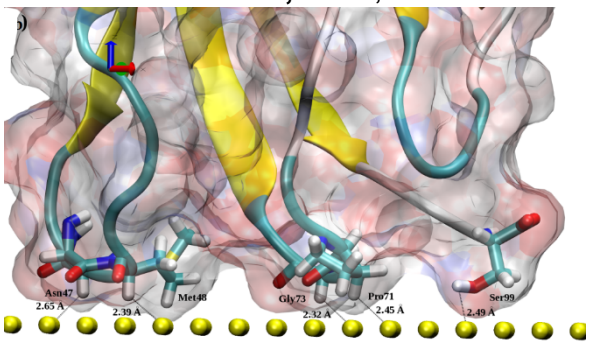
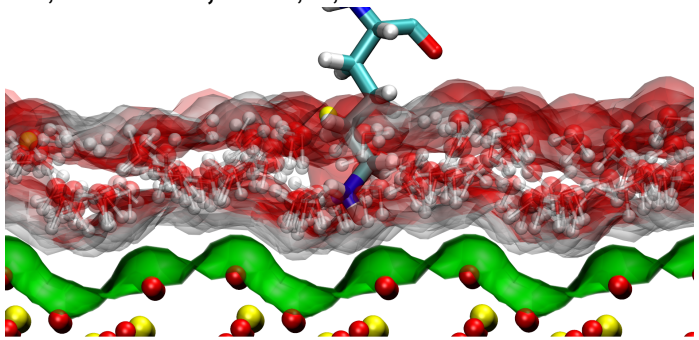
Results

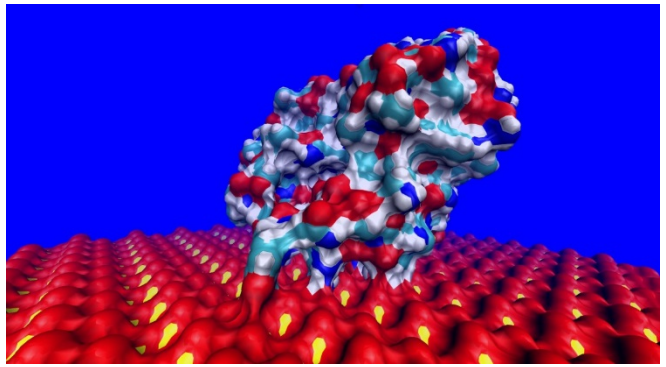
- ✓Details of HEWL, $FN^{III}9$ and BSA adsorption, diffusion and desorption (MD + zeta-potential, wettability angle, DLS, MP-SPR)

  Mol. Sim., 2009; **J. Phys. Chem. B., 2009**, 113, 12189-12200; **Langmuir 2010**, 26, 7690-7694; **Langmuir 2010**, 26, 15954-15965; **J. Phys. Chem. B., 2011**, 115, 8891-8900; **Langmuir 2012**, 28, 15577-15585; **J. Phys. Chem B., 2014**, 118, 9900-9908; **PCCP, 2015**, 17, 24070-24077; **J.Phys. Chem. B, 2016**,120-10463-10468; **RSC Adv., 2016**, 6, 73709-73716

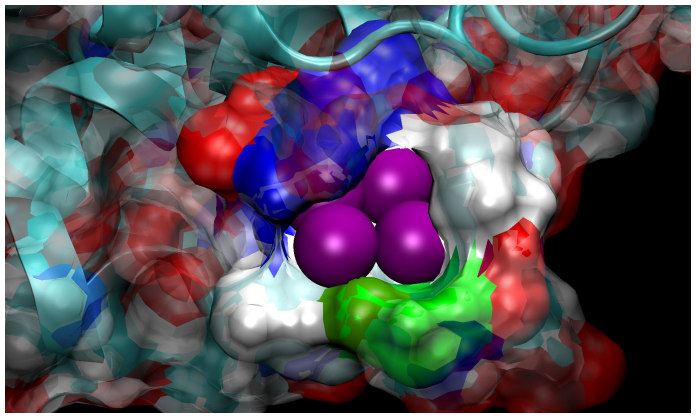








- ✓Gold NP nucleation sites on BSA (MD +fluorescence); **PCCP, 2015**,17,21935-21941



- ✓"Big protein"; surface; NPs

  Publications expected soon

- ✓MD to explain fluorescence decays

  Methods Appl. Fluoresc.,2013, 1, 015006; others expected soon

Achievements and Needs

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Achievements

✓Excellent agreement with experimental data

✓Numerous articles published in high-impact factor journals, high citation rate (in average 17 citations per paper, max. 50)

Needs

✓At least 0.5M CPU hours per paper

✓To continue the research I need to have an access to HPC

Total CPU used:

~4M CPU hours on ARCHIE-WeSt

~3M on local Strathclyde HPC

Results were obtained using the EPSRC funded ARCHIE-WeSt High Performance Computer (www.archie-west.ac.uk). EPSRC grant no. EP/K000586/1

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