

Nuno Azoia
nazoia@ceb.uminho.pt

Artur Cavaco-Paulo
artur@deb.uminho.pt

Fine and coarse-grain simulations by molecular dynamics of protein and biological interfaces



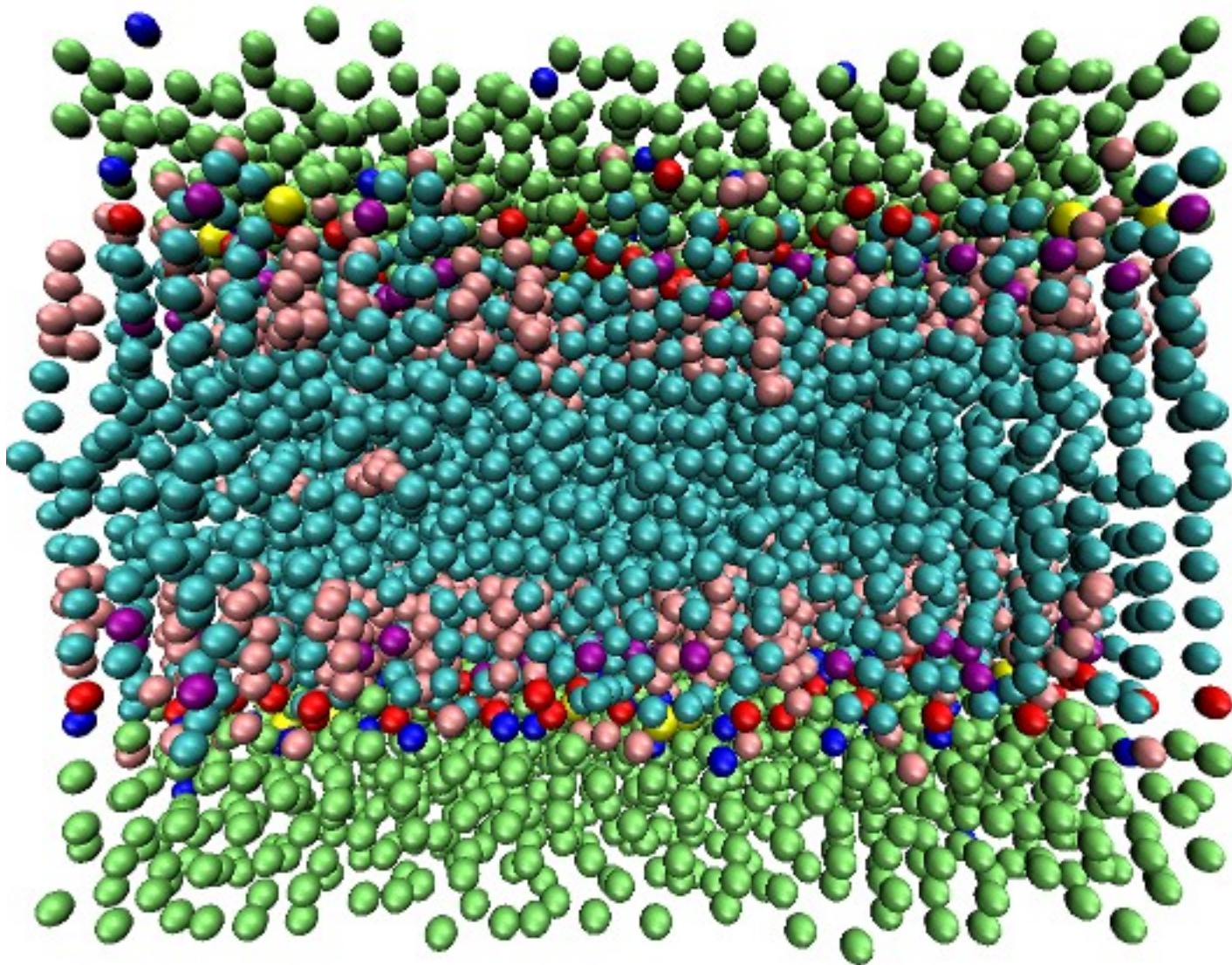
Universidade do Minho



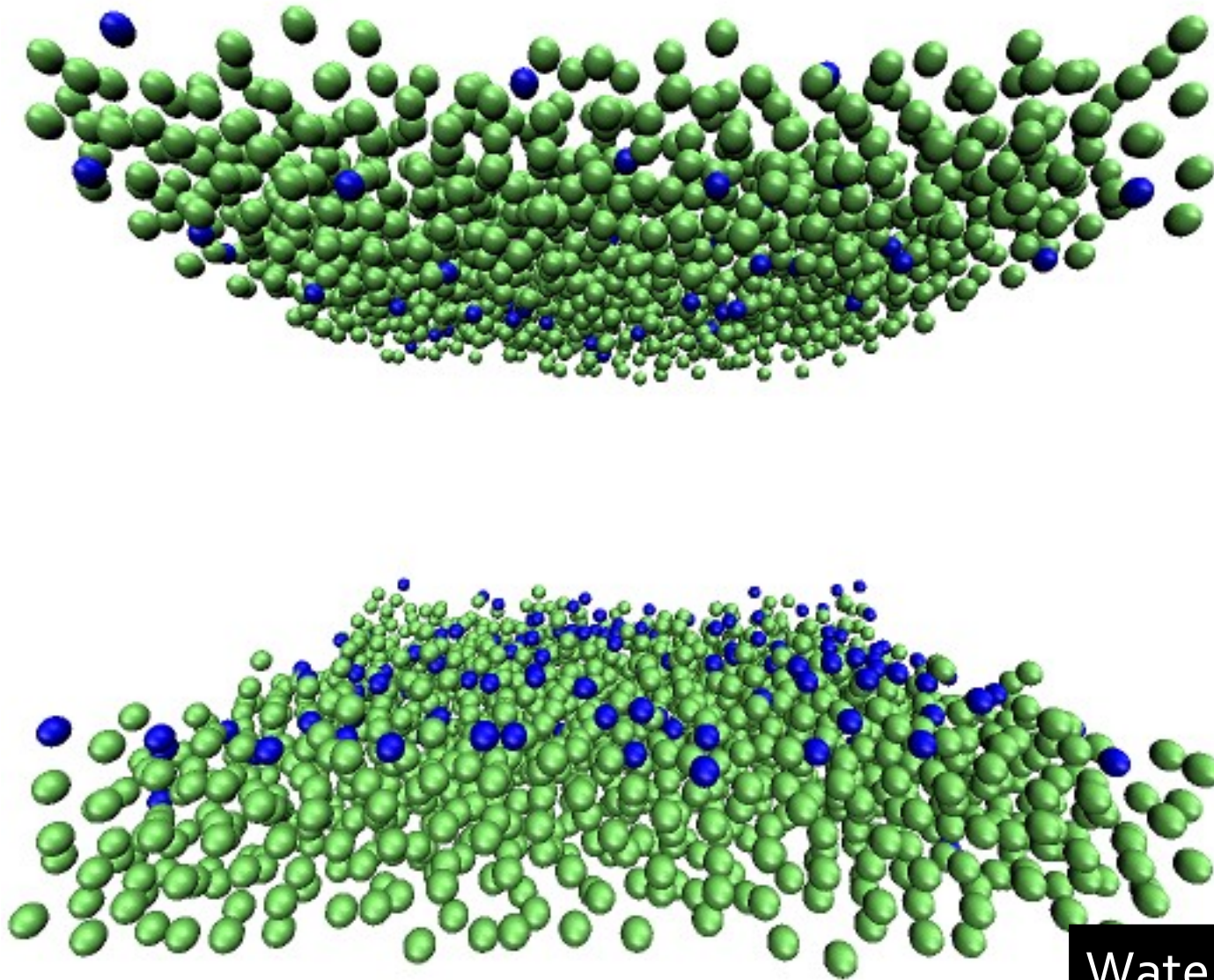
Braga, November 05, 2013

Application of molecular dynamics

Skin Model

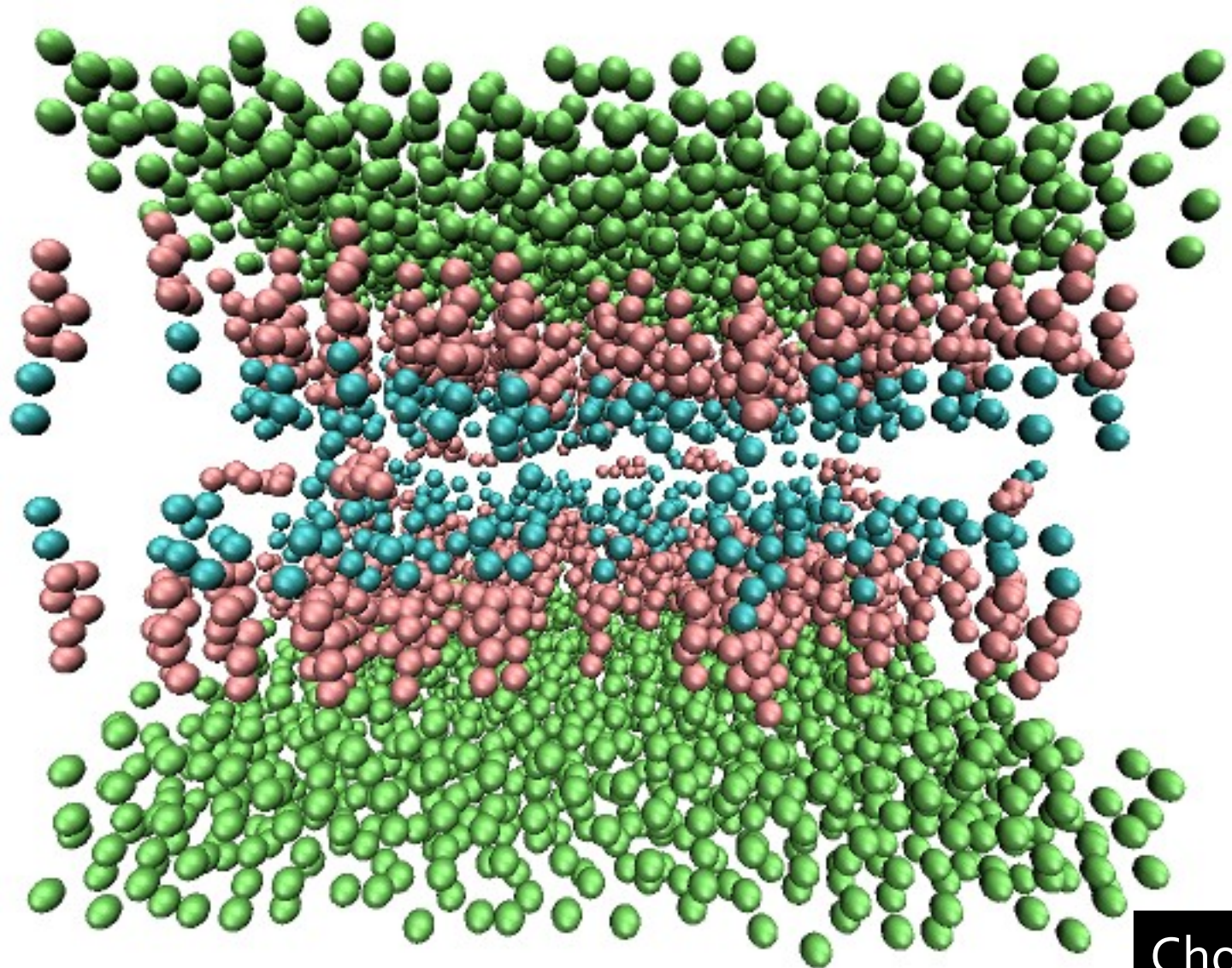


Skin Model



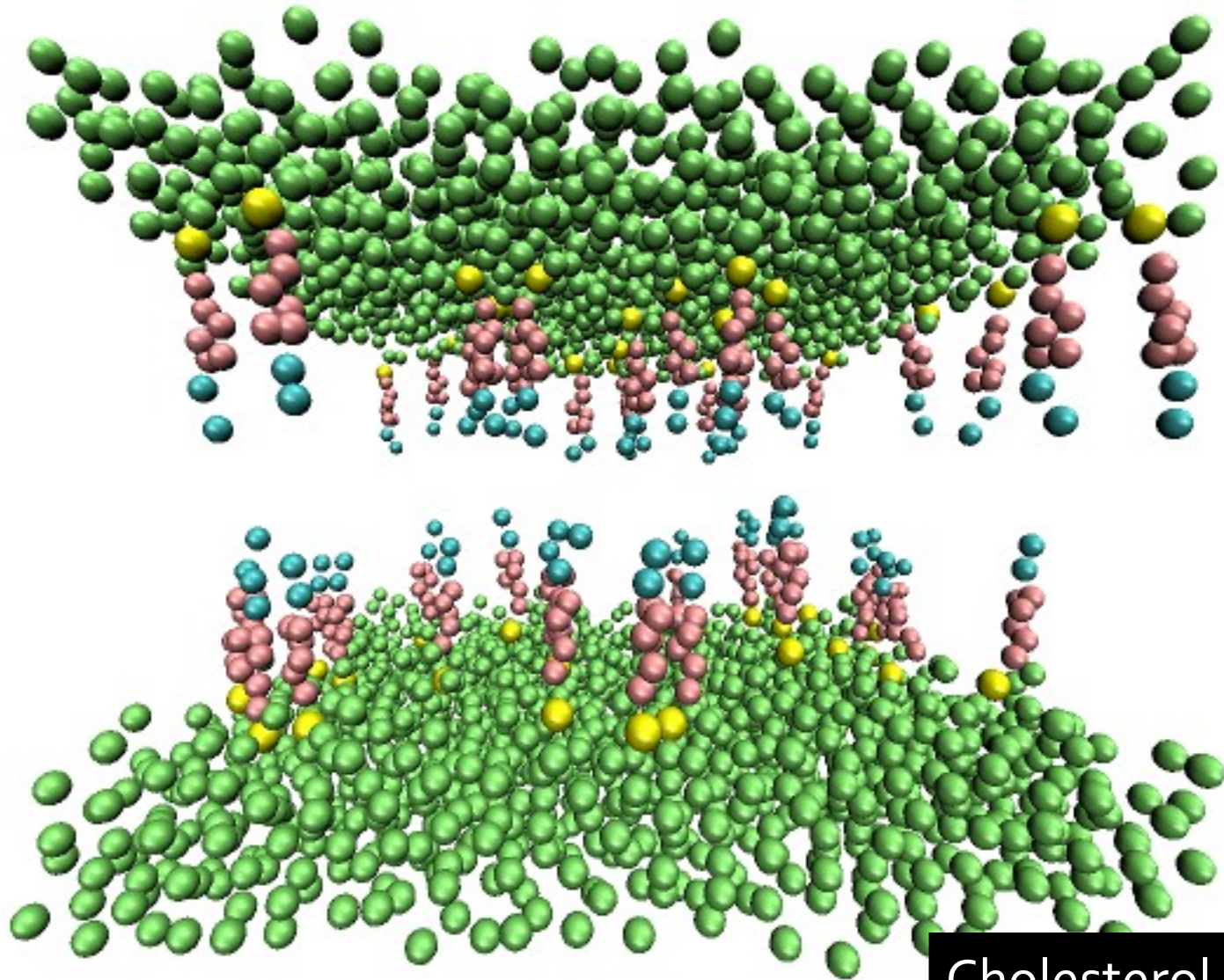
Water and ions

Skin Model

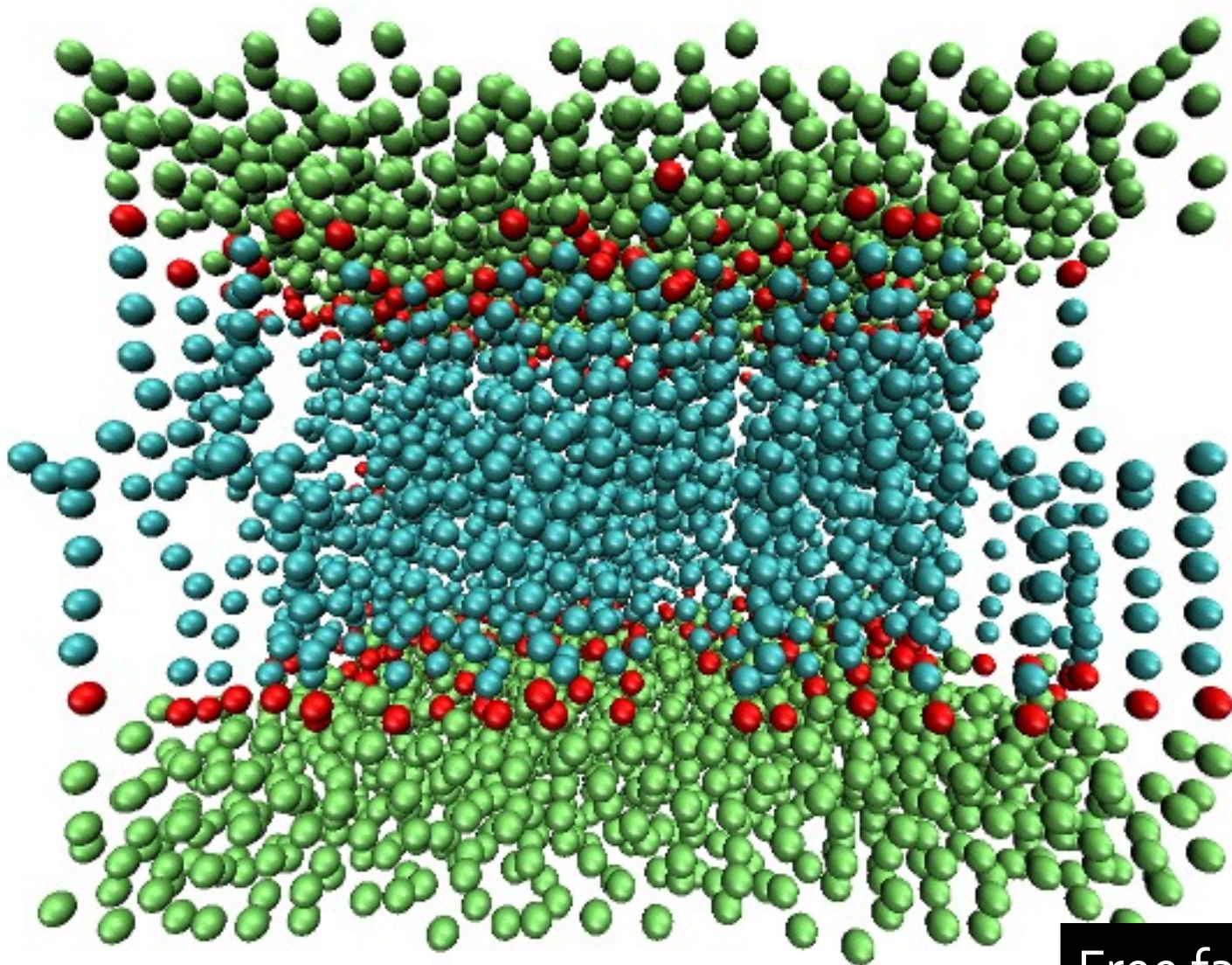


Cholesterol

Skin Model

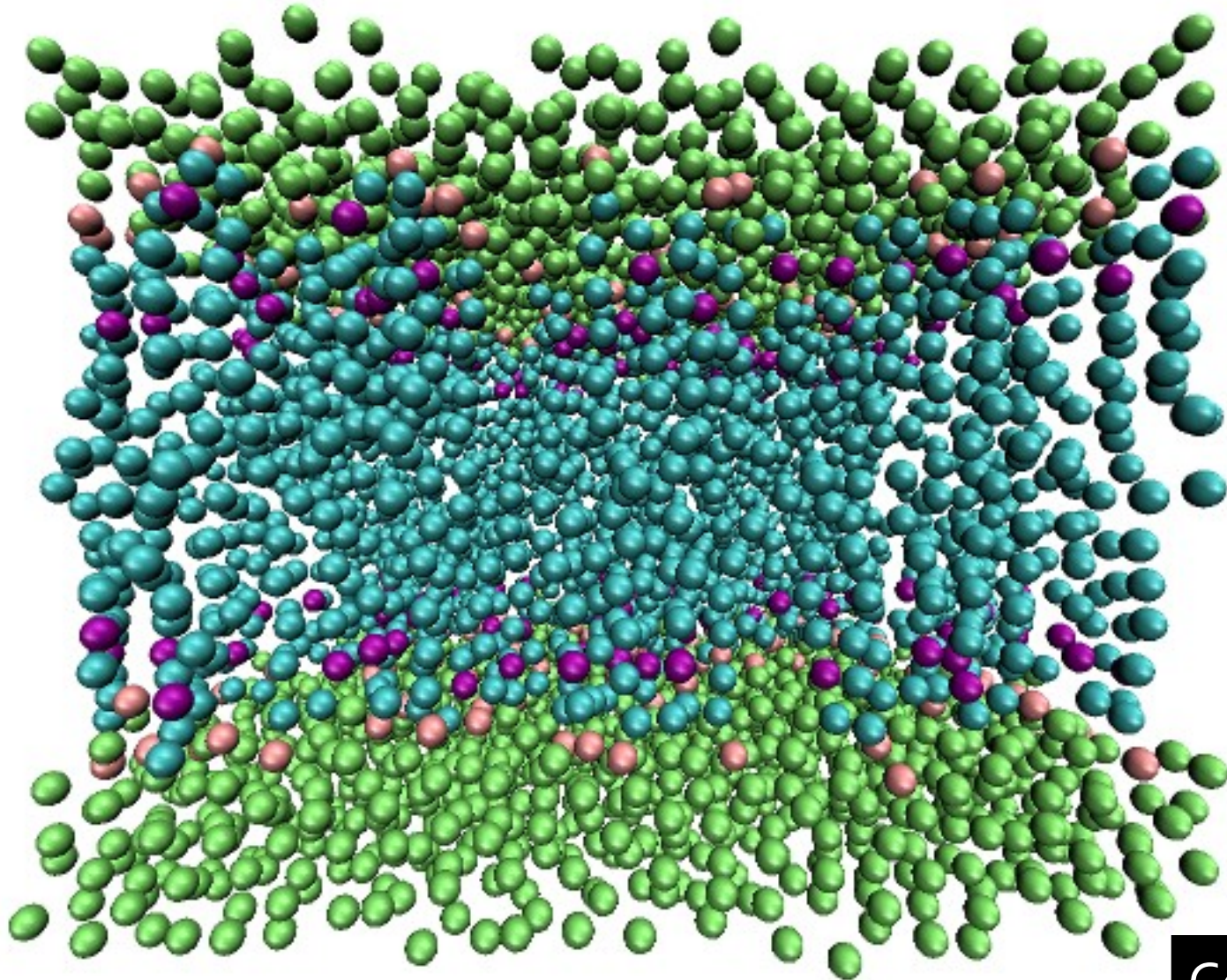


Skin Model



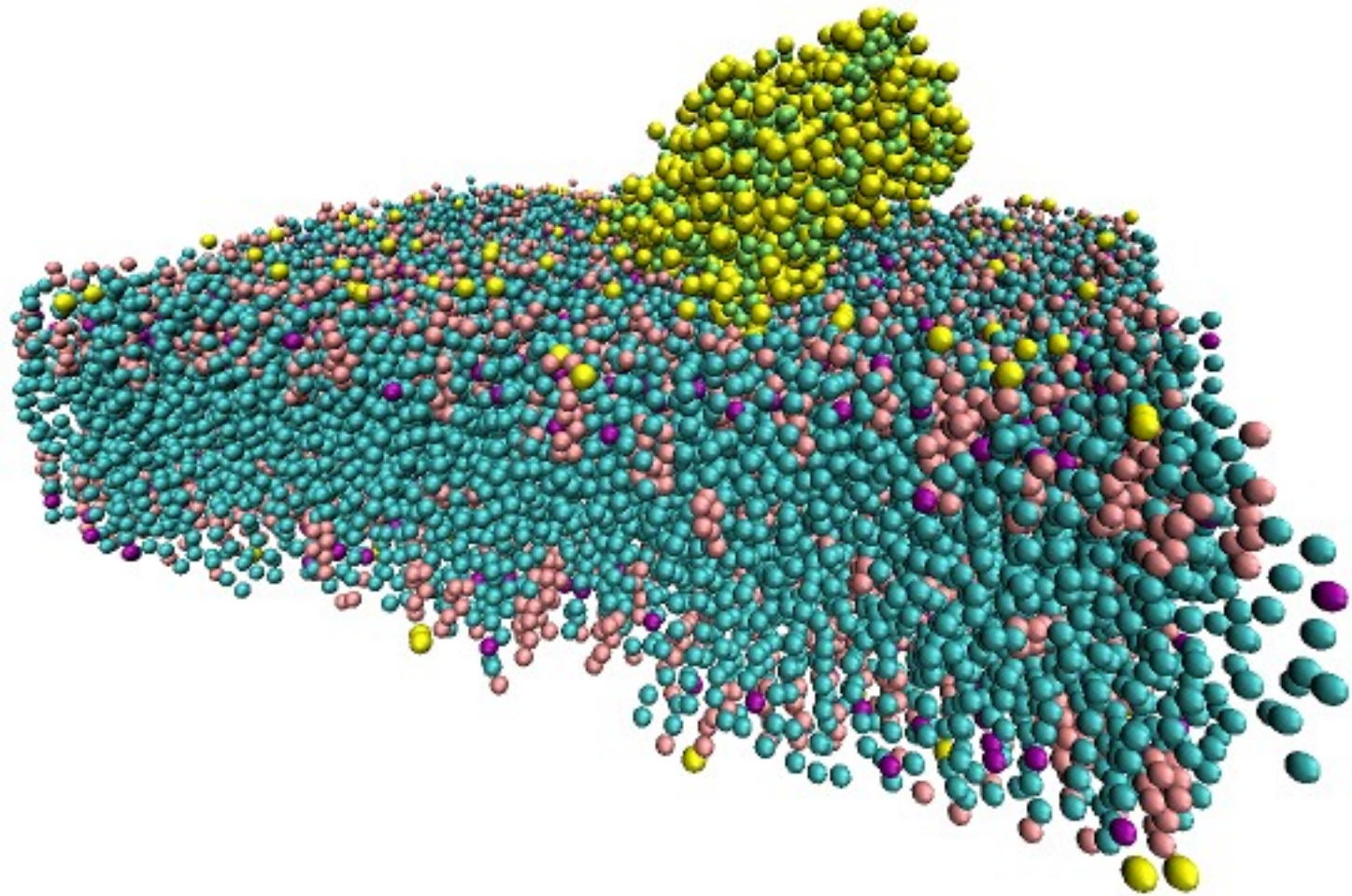
Free fatty acids

Skin Model



Ceramides

Skin and BSA



Skin and one POPC-CHOL Liposome



Contents lists available at SciVerse ScienceDirect

Colloids and Surfaces B: Biointerfaces

journal homepage: www.elsevier.com/locate/colsurfb

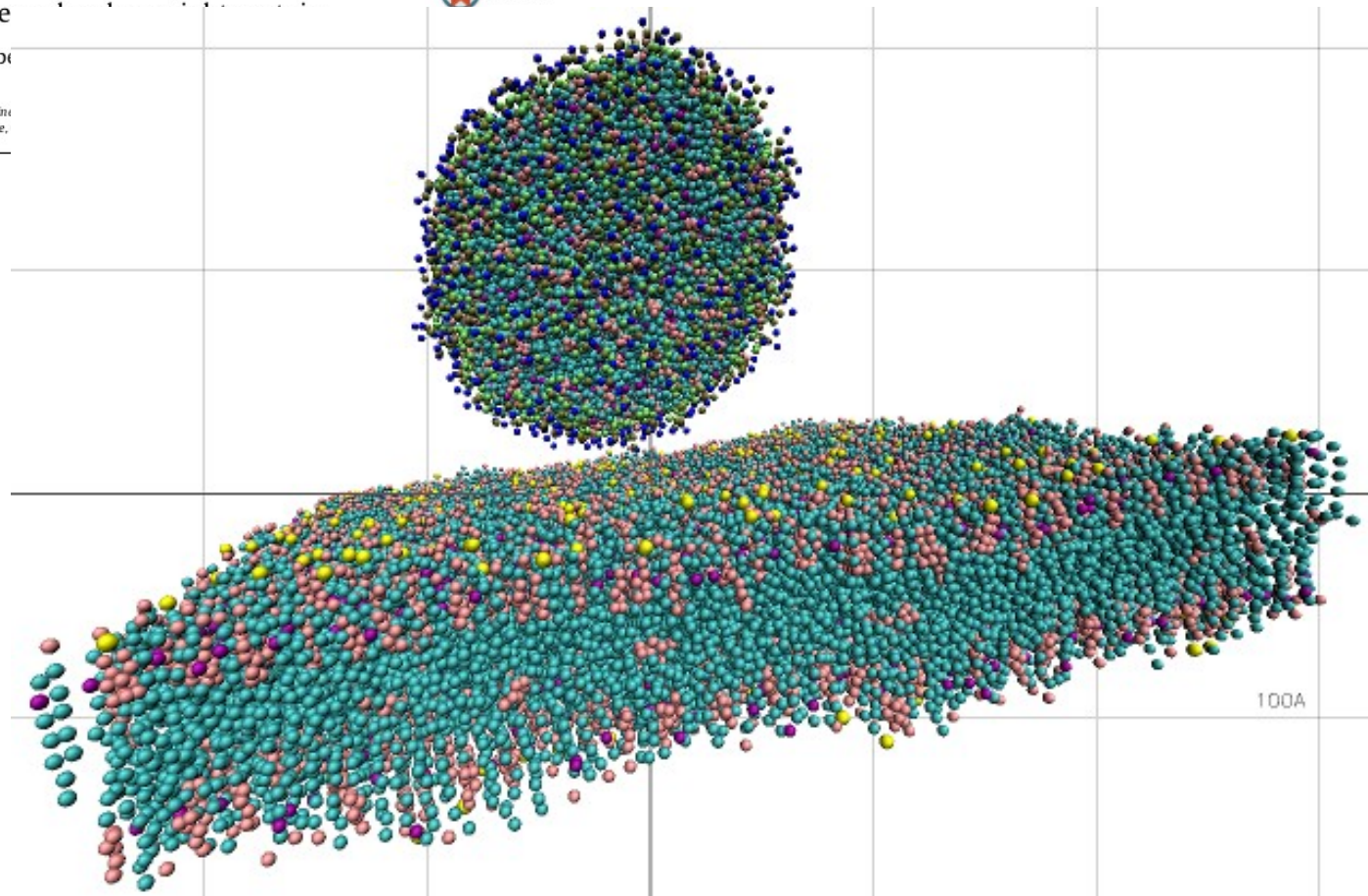


In vitro and computational studies of transdermal perfusion of nanoformulations containing a large

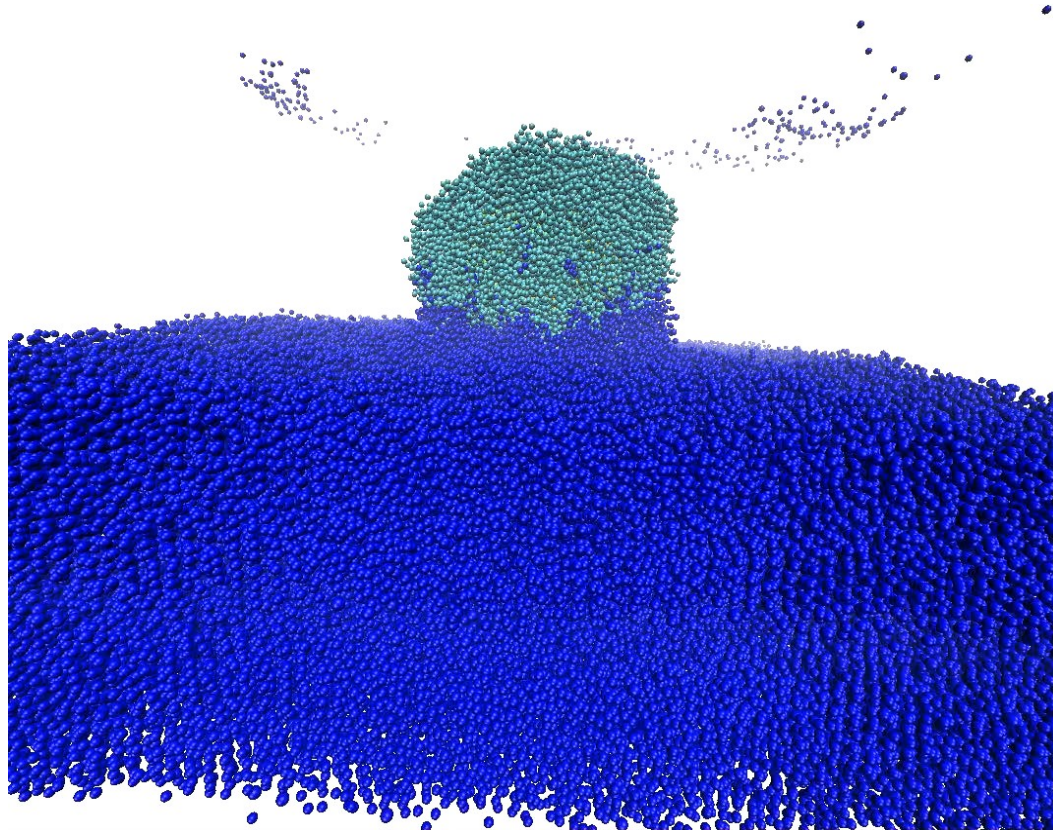
Madalena Martins^a, Nuno G. Azoia^a, Artur Ribeiro^a,
Carla Silva^a, Artur Cavaco-Paulo^{a,*}

^a IBB - Institute for Biotechnology and Bioengineering, Centre of Biological Engineering

^b Department of Chemistry, University of Cambridge, Lensfield Road, Cambridge.



Molecular Dynamics



Other applications in our lab



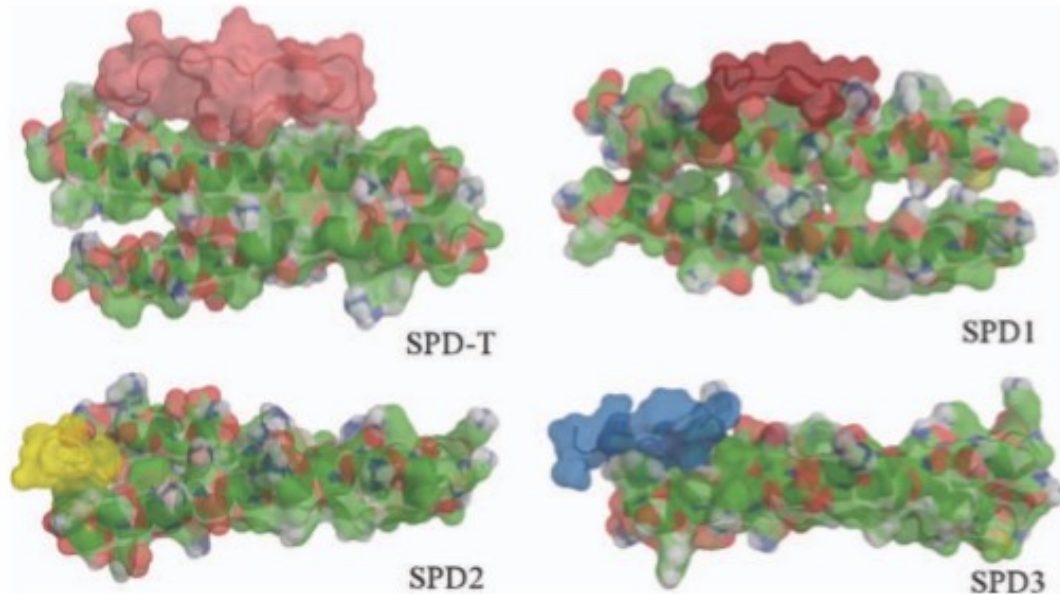
Molecular modeling of hair keratin/peptide complex: Using MM-PBSA calculations to describe experimental binding results

Nuno G. Azoia,¹ Margarida M. Fernandes,¹ Nuno M. Micaêlo,²
Cláudio M. Soares,³ and Artur Cavaco-Paulo^{1*}

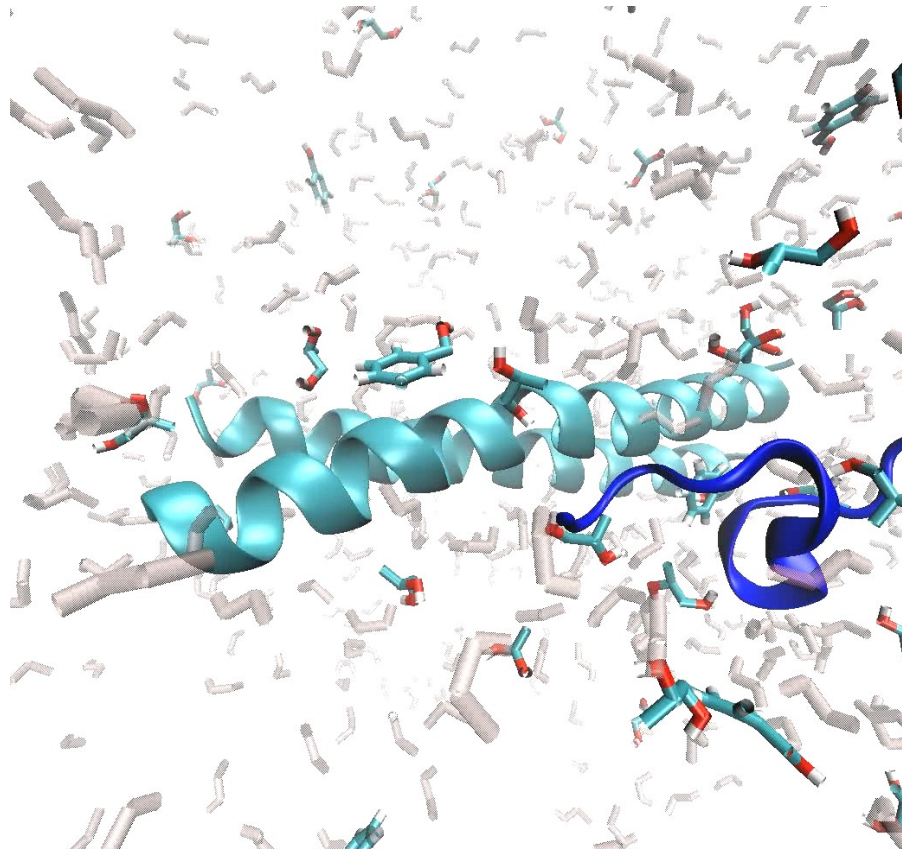
¹Departamento de Engenharia Têxtil, Universidade do Minho, Campus de Azurém, 4800-058 Guimarães, Portugal

²Chemistry Center, Minho University, Campus Gualtar, 4710-057 Braga, Portugal

³Instituto de Tecnologia Química e Biológica, Universidade Nova de Lisboa, Portugal



Other applications in our lab



Other applications in our lab

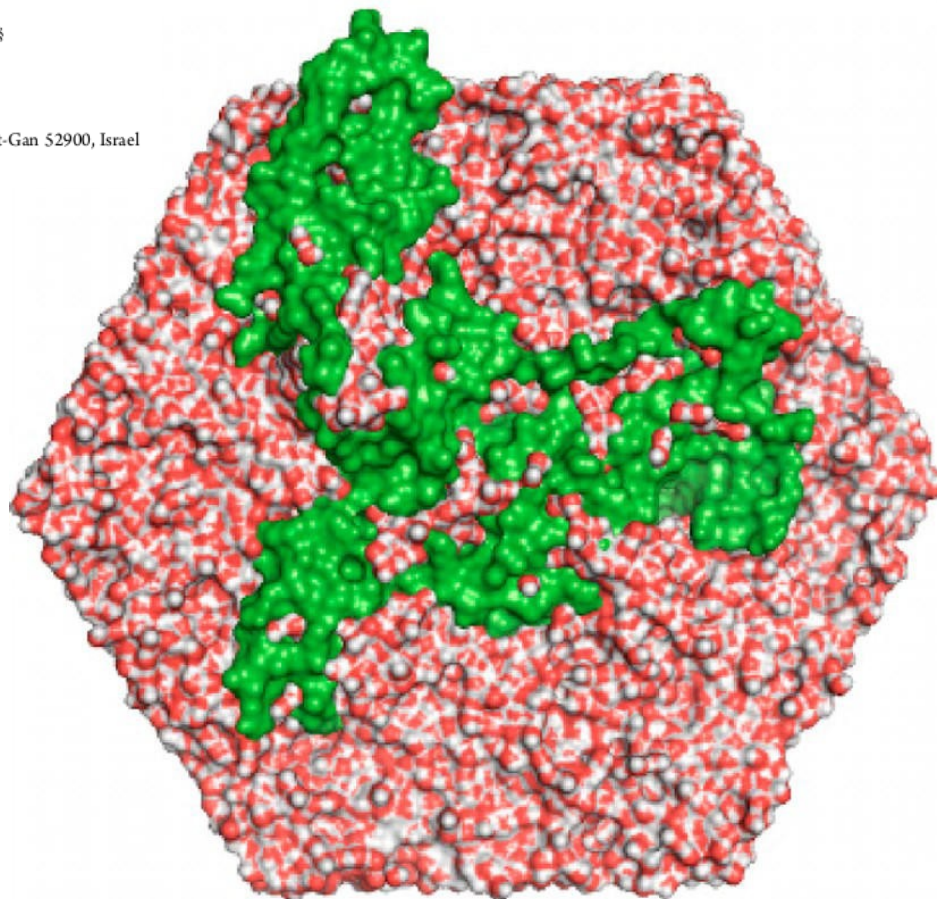
Insights on the Mechanism of Formation of Protein Microspheres in a Biphasic System

Raquel Silva,[†] Helena Ferreira,[†] Nuno G. Azoia,[†] Ulyana Shimanovich,[‡] Giuliano Freddi,[§] Aharon Gedanken,[‡] and Artur Cavaco-Paulo^{*,†}

[†]Department of Textile Engineering, University of Minho, Campus de Azurém, 4800-058, Guimarães, Portugal

[‡]Laboratory for Nanomaterials, Centre for Advanced Materials and Nanotechnology, University of Bar-Ilan, Ramat-Gan 52900, Israel

[§]Silk Research Institute, Via Giuseppe Colombo 83, 20133 Milan, Italy



Other applications in our lab



Contents lists available at SciVerse ScienceDirect

Colloids and Surfaces B: Biointerfaces

journal homepage: www.elsevier.com/locate/colsurfb

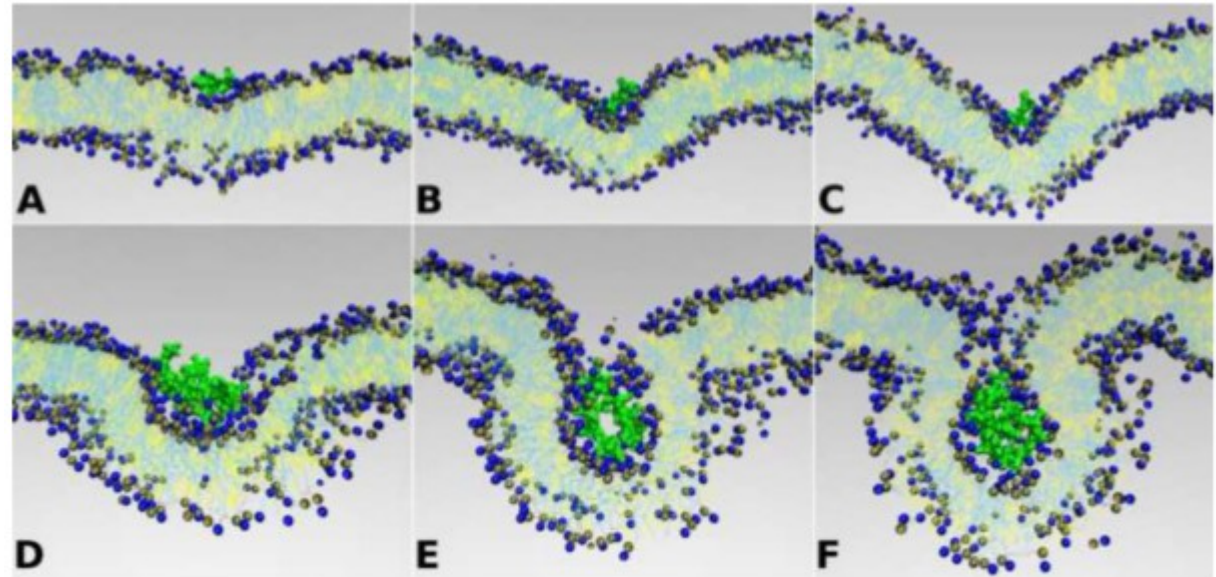


The activity of LE10 peptide on biological membranes using molecular dynamics, in vitro and in vivo studies

Egito Antunes^a, Nuno G. Azoia^a, Teresa Matamá^{a,b}, Andreia C. Gomes^b, Artur Cavaco-Paulo^{a,*}

^a Biological Engineering Department, University of Minho, Campus of Gualtar, 4710-057 Braga, Portugal

^b Molecular and Environmental Biology Centre (CBMA), Department of Biology, University of Minho, Campus of Gualtar, 4710-057 Braga, Portugal



Other applications in our lab



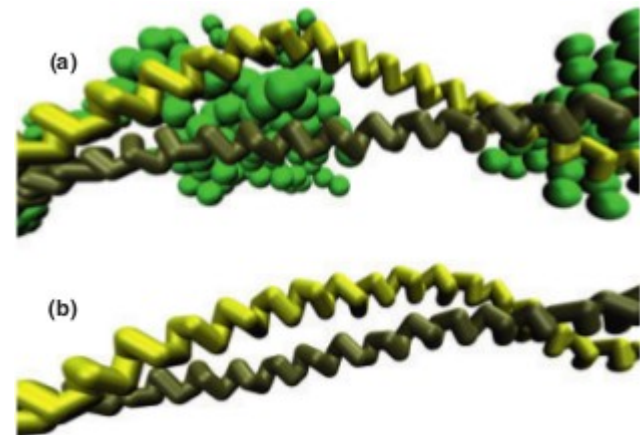
Keratins and lipids in ethnic hair

C. F. Cruz*, M. M. Fernandes*, A. C. Gomes[†], L. Coderch[‡], M. Martí[‡], S. Méndez[‡], L. Gales[§], N. G. Azoia*, U. Shimanovich* and A. Cavaco-Paulo*

*Biological Engineering Department, Campus of Gualtar, University of Minho, 4710-057 Braga, Portugal, [†]Department of Biology, Centre of Molecular and Environmental Biology (CBMA), Campus of Gualtar, University of Minho, 4710-057, Braga, Portugal, [‡]IQAC (CSIC), Jordi Girona 18-26, 08034, Barcelona, Spain and [§]INEB, Rua do Campo Alegre, N 823, 4150-180, Porto, Portugal

Received 06 August 2012, Accepted 17 December 2012

Keywords: ethnicity, hair, keratin, lipid, protein



Molecular dynamics principles

Molecular Dynamics Principles



The Nobel Prize in Chemistry 2013

Martin Karplus, Michael Levitt, Arieh Warshel

The Nobel Prize in Chemistry 2013



© Harvard University

Martin Karplus



Photo: © S. Fisch

Michael Levitt



Photo: Wikimedia Commons

Arieh Warshel

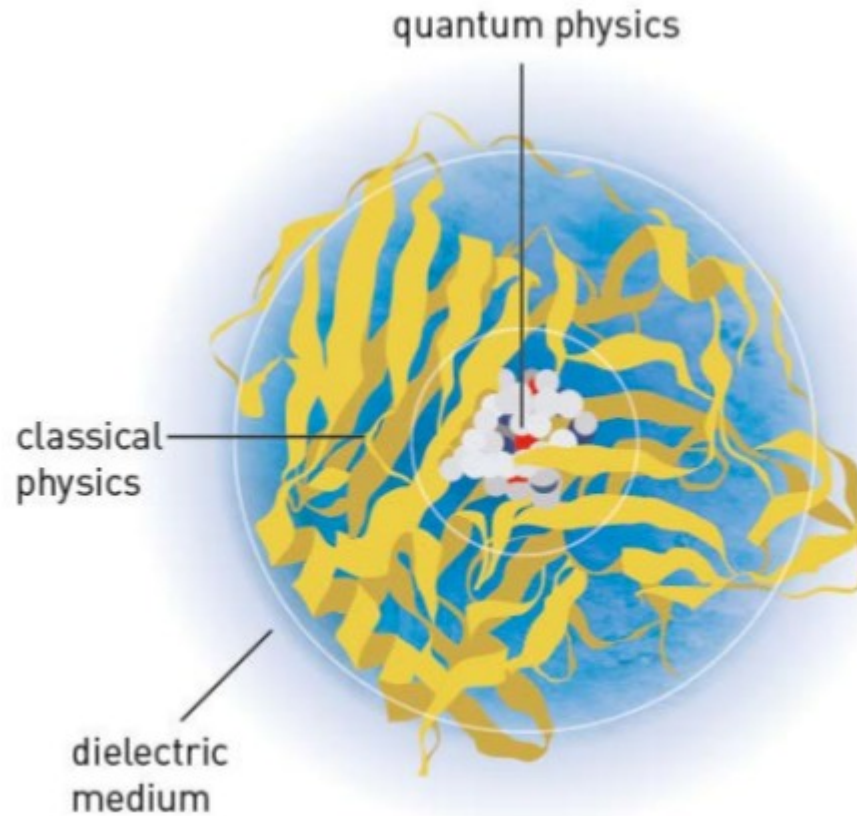
The Nobel Prize in Chemistry 2013 was awarded jointly to Martin Karplus, Michael Levitt and Arieh Warshel *"for the development of multiscale models for complex chemical systems"*.

Molecular Dynamics Principles

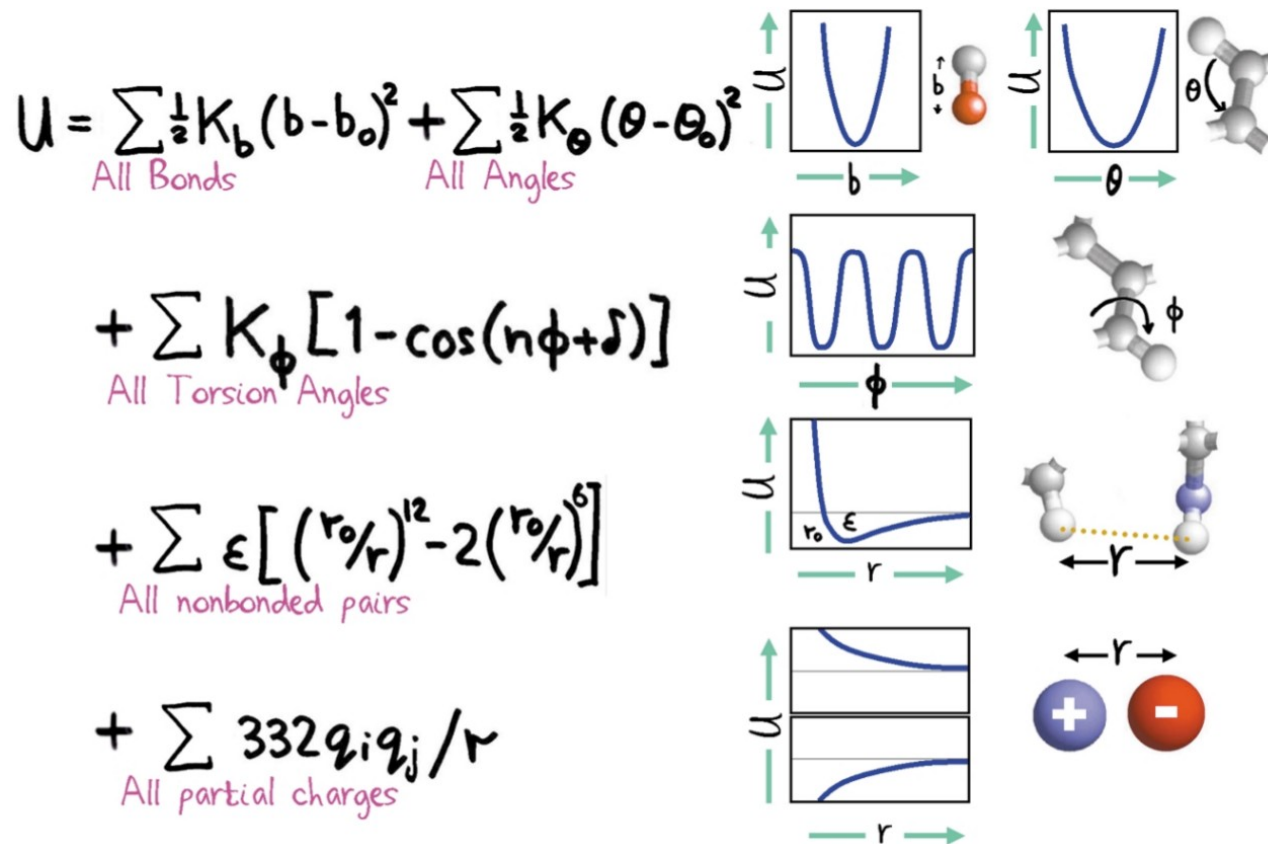


Figure 2. Newton and Schrödinger's cat. Previously, classical physics and quantum chemistry belonged to rivalling worlds. The Nobel Laureates in Chemistry 2013 have opened a gate between those worlds and have brought about a flourishing collaboration.

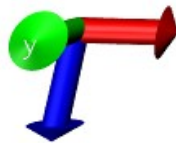
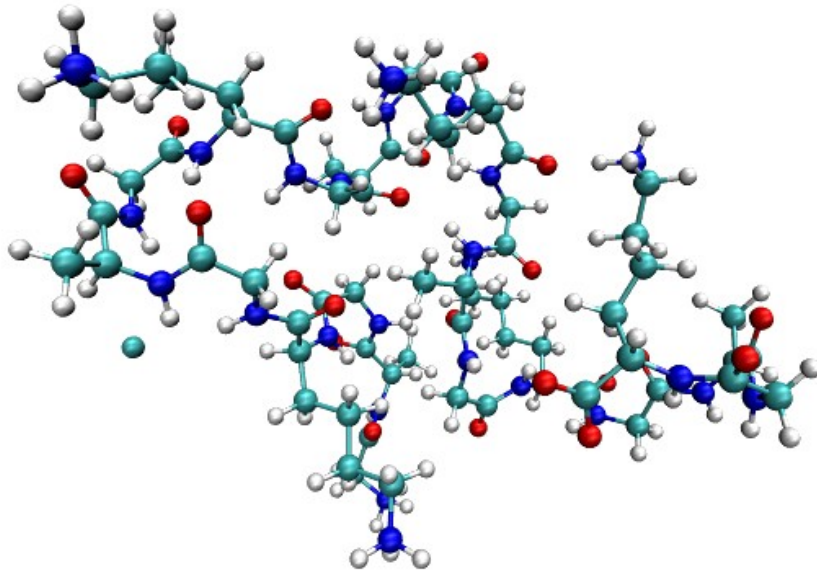
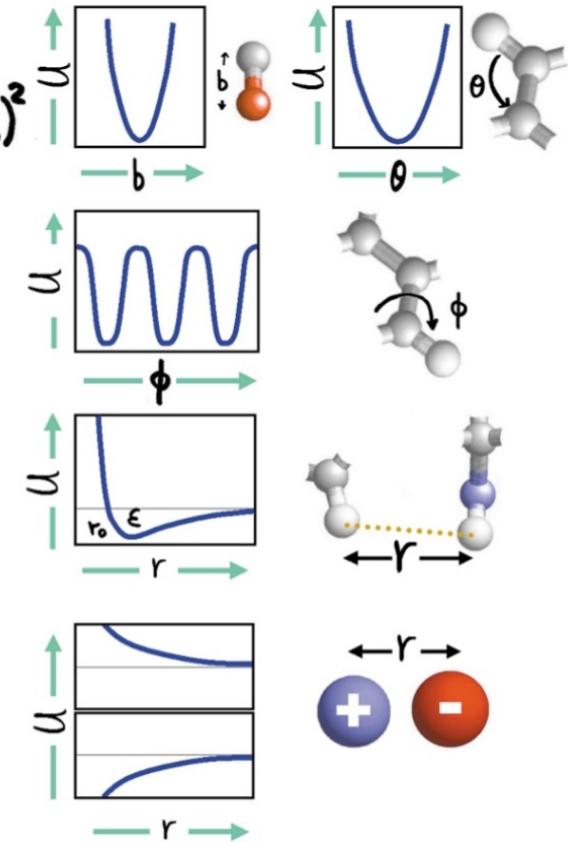
Molecular Dynamics Principles



Potential energy of the system

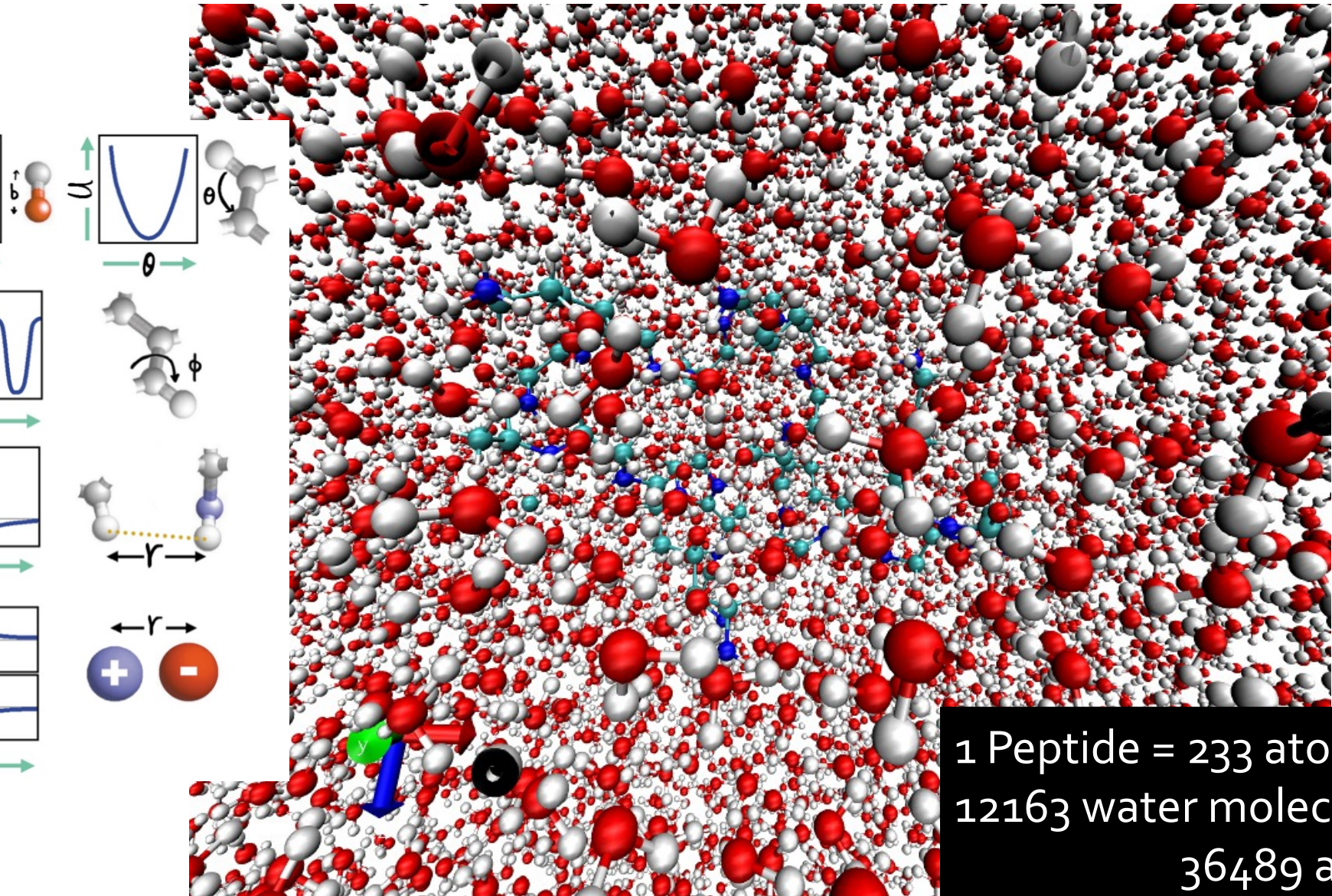


Example – one small peptide



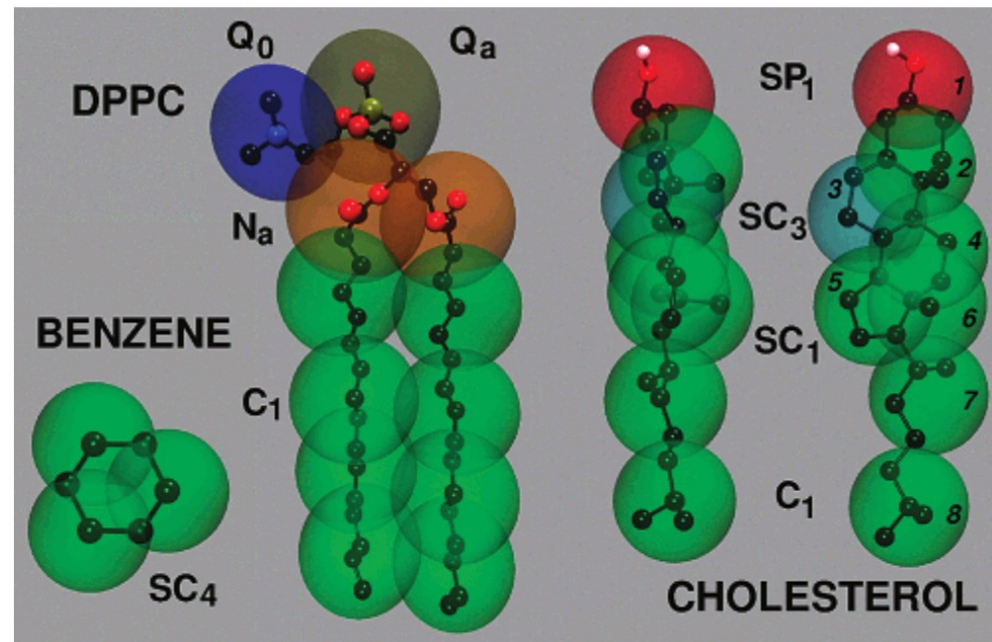
1 Peptide = 233 atoms

Example – one small peptide



Simplifications

- United atoms
- Single Point Charge water
- Coarse grained models
- Implicit solvent simulations



Parallelization

- The simulation box is divided in smaller problems
- Because the system is dynamic, the small problems are not independent
- By experience, coarse grained models are more difficult to parallelize, probably because the particles have a higher mobility