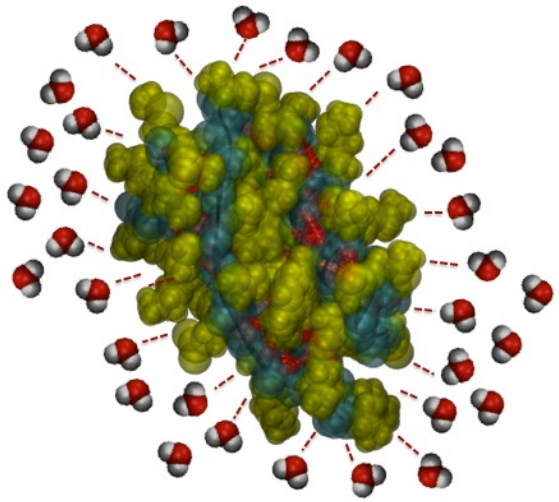
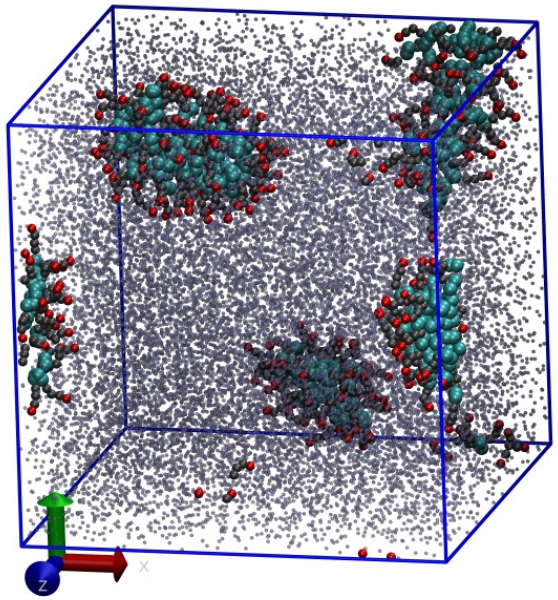
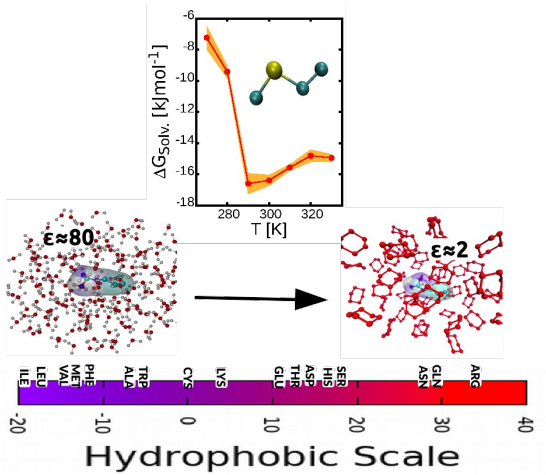
Ca' Foscari University of Venice

Can Life exist without water?
A data driven approach

www.unive.it







Achille Giacometti

ESA_LAB Venice 8 May 2023

Ca' Foscari University of Venice

ECLT European Centre for Living Technology

www.unive.it

European Centre for Living Technology (ECLT)

www.eclt.eu

@ECLT Venice

2004: The Foundation

Project Information

PACE

Grant agreement ID: 002035

Start date 1 April 2004

End date 30 June 2008

Funded under FP6-IST

Overall budget € 7 928 932

EU contribution € 6 605 000

Coordinated by RUHR-UNIVERSITAET BOCHUM

Germany

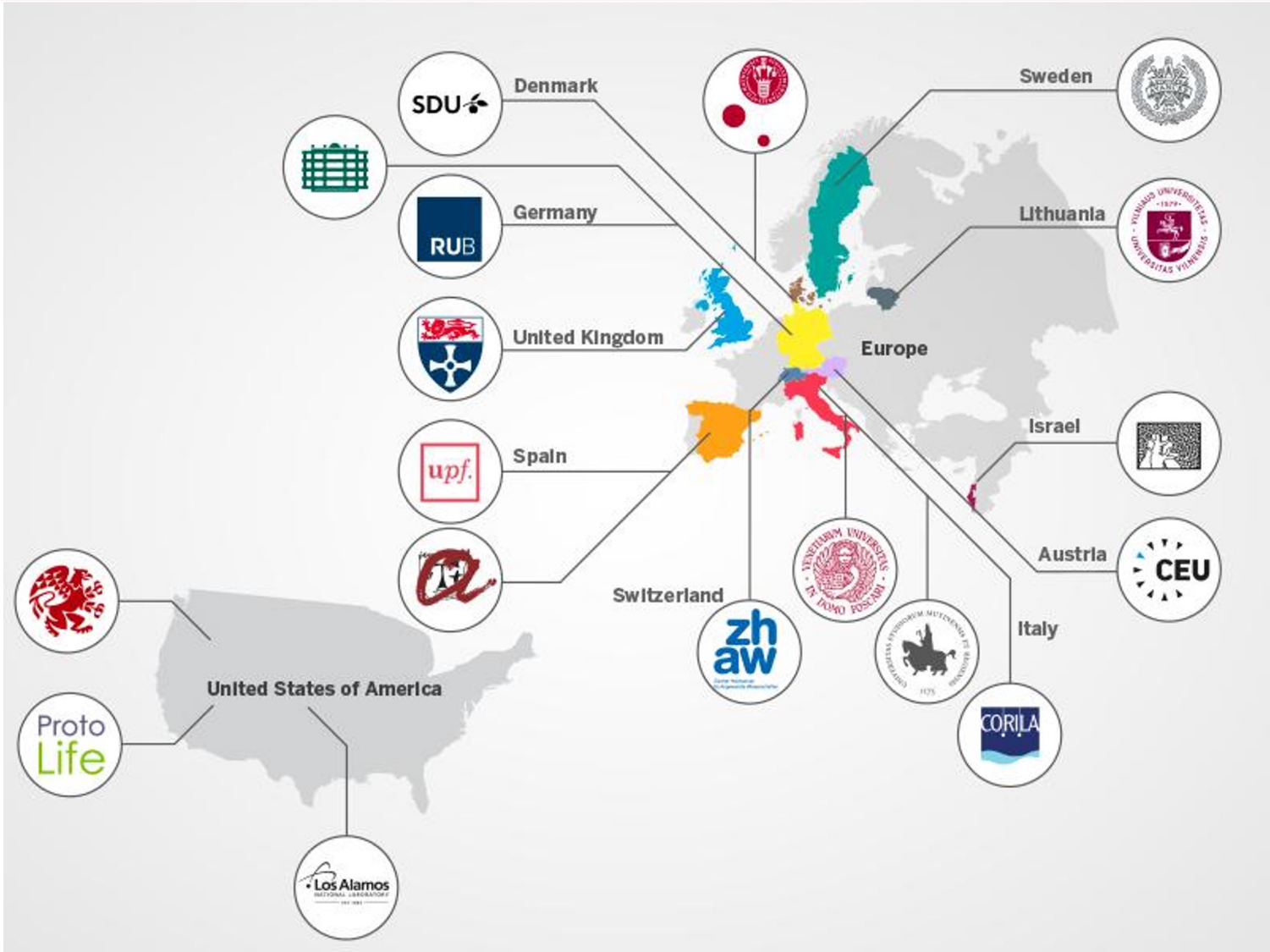
Programmable Artificial Cell Evolution (PACE)

Objectives

The integrated project PACE will explore the utilization of the simplest technically feasible elementary living units (artificial cells much simpler than current cells) to build evolvable complex information systems. We will create, analyse and investigate the applications of such systems that process information by self-organization starting at molecular scales. We will also determine whether life-like properties are necessary for computational systems to be fully robust and adaptive and investigate the tension between evolvable living autonomy and programmable utilization.

European Centre for Living Technology (ECLT)

ECLT is a **consortium** of **18** Universities, Laboratories, Research Centres, European and extra-European.



ECLT Members

HOST INSTITUTION

University Ca' Foscari of Venice
Italy

FOUNDING MEMBERS

Ruhr-Universitaet Bochum
Germany

University Ca' Foscari of Venice
Italy

University of Copenhagen
Denmark

Chalmers Tekniska Hogskola
Sweden

Universitat Pompeu Fabra
Spain

Vilnius University Institute of Theoretical Physics and Astronomy
Lithuania

ProtoLife
USA

University of Southern Denmark
Denmark

Reed College
USA

Los Alamos National Laboratory
USA

OTHER MEMBERS

Newcastle University
UK

Weizmann Institute of Science
Israel

CORILA
Italy

Università di Modena e Reggio Emilia
Italy

Zurich University of Applied Sciences School of Engineering
Switzerland

University of Rovira I Virgili (URV)
Spain

Central European University (CEU)
Austria

Chemnitz University of Technology
Germany

Ca' Foscari University of Venice

ECLT European Centre for Living Technology

www.unive.it

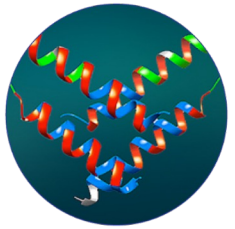
History

Founded in **2004** the **European Centre for Living Technology** by an initial funding through the **EU project PACE** (*Programmable Artificial Cell Evolution, FP6*), is an international and interdisciplinary research centre hosted by **Ca' Foscari University of Venice** and established as an inter-university consortium, currently involving **18 European and extra-European institutional affiliates**.

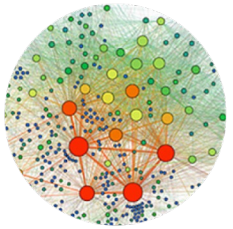
The Centre is devoted to the study of technologies that exhibit life-like properties including self-organization, adaptability and the capacity to evolve.

Research Units

Artificial Intelligence



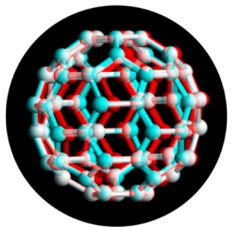
Bioinspired design



Science of Complexity

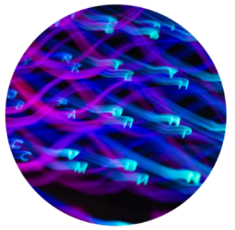
Arts and Complexity

Neuroscience



Artificial Life

Living Technology



Solutions

ECLT Projects

Total funded projects from ECLT's foundation **(2004 - 2022):**

34 with a total budget of about

~46 /7.9 M €

(including Research contracts - "conto terzi")

In the last few years **(2019 - 2023):**

42 submitted proposals, of which:

12 accepted for funding

ECLT Ongoing Projects

DC-ren
Drug combinations for rewriting trajectories of renal pathologies in type II diabetes

GLOBAL_AT_VENICE
A Research and Training for Global Challenges
Cofund Fellowship Programme

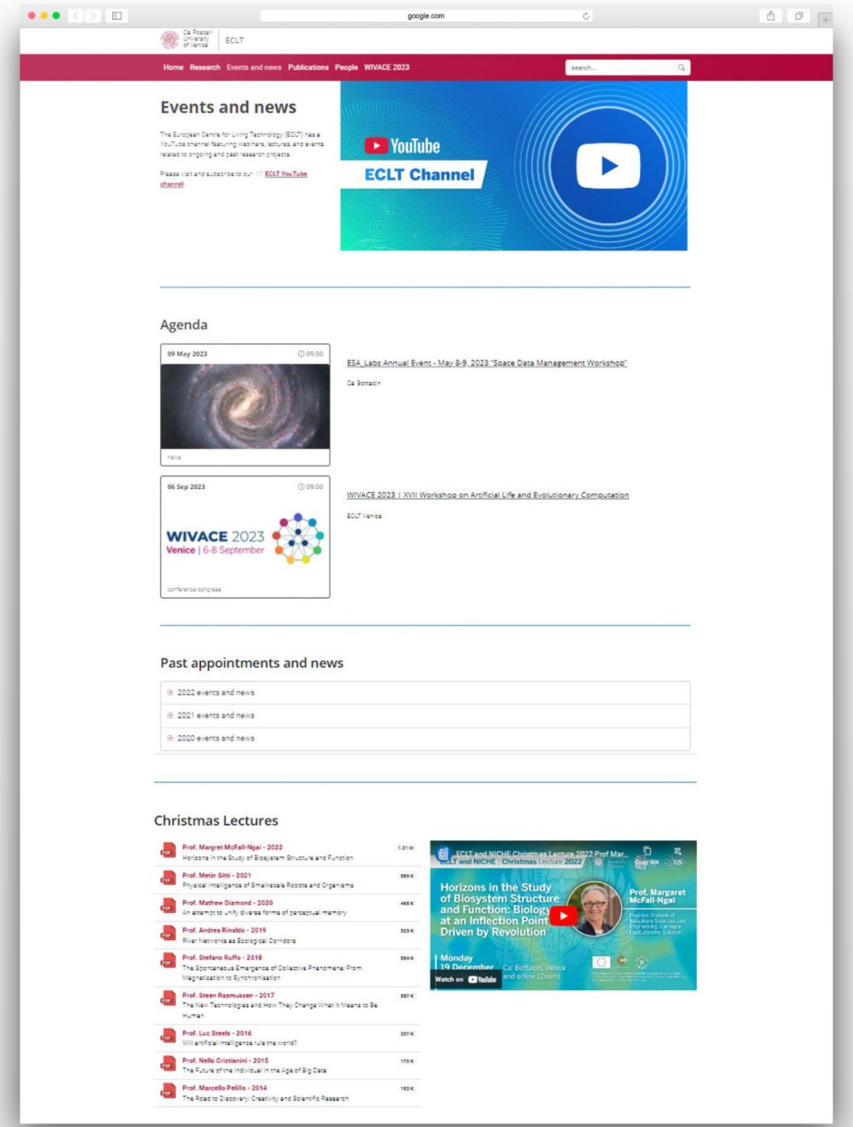
ELISE
European Learning and Intelligent Systems Excellence

NODES
NODES European Narratives Observatory to fight Disinformation post COVID-19

REXlearn
Reliable and Explainable Adversarial Machine Learning

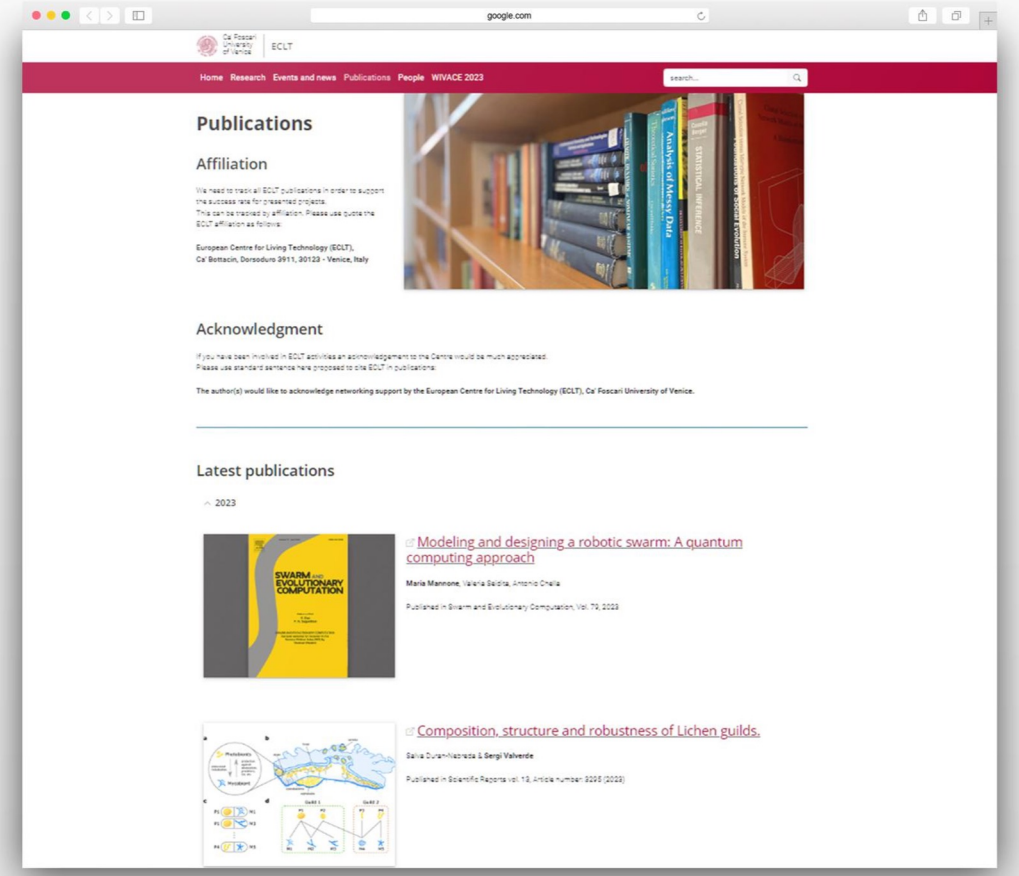
ECLT Website

- Events and news
- Christmas Lectures
- Youtube Channel



ECLT Website

- Publications with ECLT affiliation or acknowledgment



ECLT Governance | Board of Directors |

Rudolf M. Füchslin
Professor for Applied Complex Systems Sciences, Zurich University of Applied Sciences

Achille Giacometti
Full Professor of Condensed matter physics at Ca' Foscari University of Venice

Norman Packard
Founder of ProtoLife and chaos theory physicist

ECLT Governance | Science Board |

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Full Professor of Physics at Ca' Foscari and a LIMS Fellow, President of the Complex Systems Society

Harold Fellermann
Lecturer at the School of Computing, Newcastle University, England

John McCaskill
Professor of Theoretical Biochemistry (D.Phil. Oxford, 1982 in Theoretical Chemistry)

Norman Packard
Founder of ProtoLife and chaos theory physicist

Rudolf M. Füchslin
Professor for Applied Complex Systems Sciences, Zurich University of Applied Sciences

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Full professor of Complex Systems at the Department of Physics, Informatics and Mathematics - Unimore

Marco Villani
Associate professor, Università di Modena e Reggio Emilia

Ca' Foscari University of Venice

www.unive.it

Some contributions from the network

Doron Lancet (Weitzmann)

Cell Reports Physical Science

Article

Attractor dynamics drives self-repr
in protobiological catalytic network

Amit Kahana,[1,3] Lior Segev,[2] and Doron Lancet[1,4,*]

Petra Schwille (Max Planck)

CellPress

Trends in Cell Biology

Opinion

Hidden protein functions and what they may teach us

Petra Schwille[1,*] and Béla P. Frohn[1]

Ivan Gladich (Qatar)

ACS EARTH AND SPACE CHEMISTRY

http://pubs.acs.org/journal/aesccq

Article

Unexpected Behavior of Chloride and Sulfate Ions upon Surface Solvation of Martian Salt Analogue

Nicolas Fauré, Jie Chen, Luca Artiglia, Markus Ammann, Thorsten Bartels-Rausch, Jun Li, Wanyu Liu, Sen Wang, Zamin A. Kanji, Jan B. C. Pettersson, Ivan Gladich,* Erik S. Thomson,* and Xiangrui Kong*

Cite This: *ACS Earth Space Chem.* 2023, 7, 350–359 Read Online

Steen Rasmussen (Copenhagen)

Volume 25, Issue 2
Spring 2019

ARTIFICIAL LIFE

May 01 2019

An Overview of Open-Ended Evolution: Editorial Introduction to the Open-Ended Evolution II Special Issue

In Special Collection: CogNet

Norman Packard, Mark A. Bedau, Alastair Channon, Takashi Ikegami, Steen Rasmussen, Kenneth O. Stanley, Tim Taylor

Author and Article Information

Artificial Life (2019) 25 (2): 93–103.

https://doi.org/10.1162/artl_a_00291

Norman Packard (Protolife)

ACS SyntheticBiology

Cite This: *ACS Synth. Biol.* 2018, 7, 2841–2853

High-Throughput Optimization Cycle of a Cell-Fr Assembly and Protein Synthesis System

Filippo Caschera,[¶,†,‡,§] Ashty S. Karim,[¶,†,‡,§] Gianluca Gazzola,[⊥] Anne E. Norman H. Packard,[#] and Michael C. Jewett*[,†,‡,§,∥,⊥,▽,⊗]

Harold Fellerman (NewCastle)

Bioinformatics, 35(19), 2019, 3859–3860
doi: 10.1093/bioinformatics/btz131
Advance Access Publication Date: 23 February 2019
Applications Note

OXFORD

Systems biology

Easybiotics: a GUI for 3D physical modelling of multi-species bacterial populations

Jonathan Naylor, Harold Fellermann and Natalio Krasnogor*

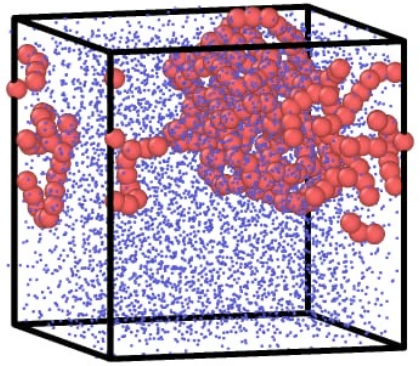
Interdisciplinary Computing and Complex BioSystems (ICOS) research group, School of Computing Science, Newcastle University, Newcastle upon Tyne NE4 5TG, UK

Ca' Foscari University of Venice

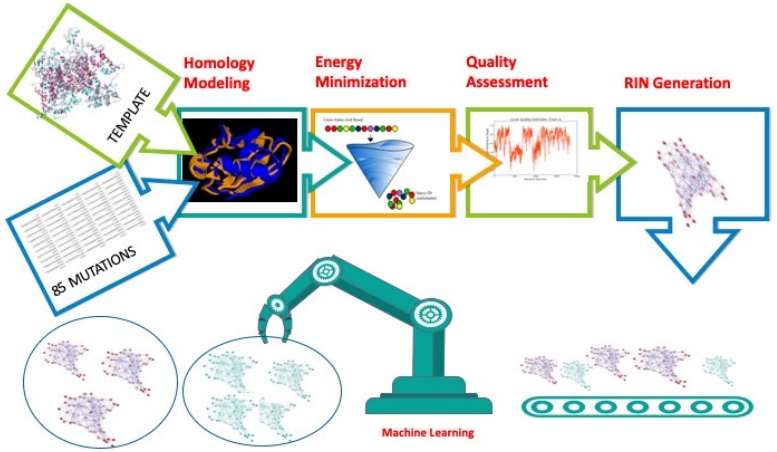
www.unive.it

Our Lab

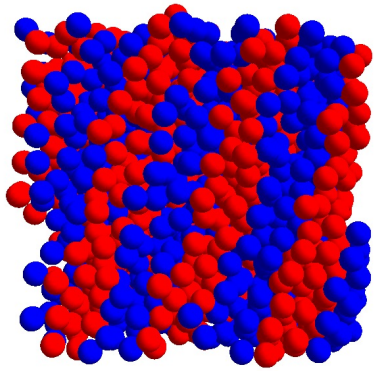
Polymers



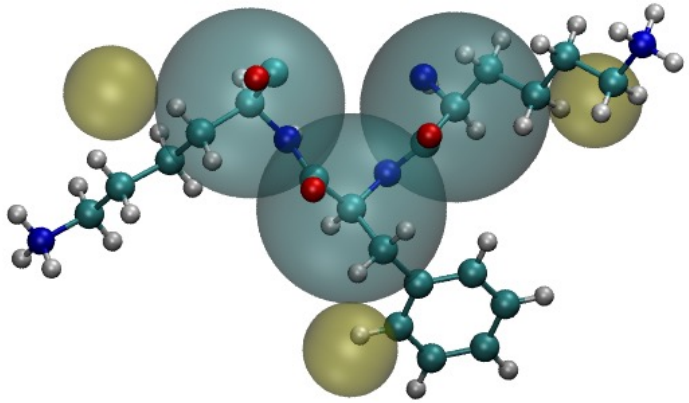
AI and Membrane Proteins



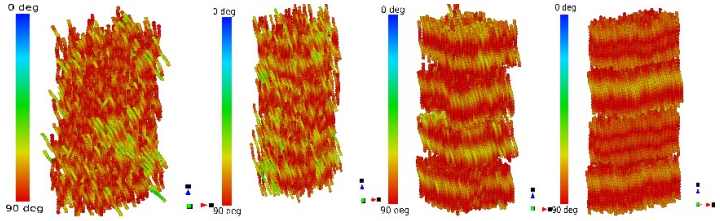
Colloids and patchy colloids



CG models for proteins

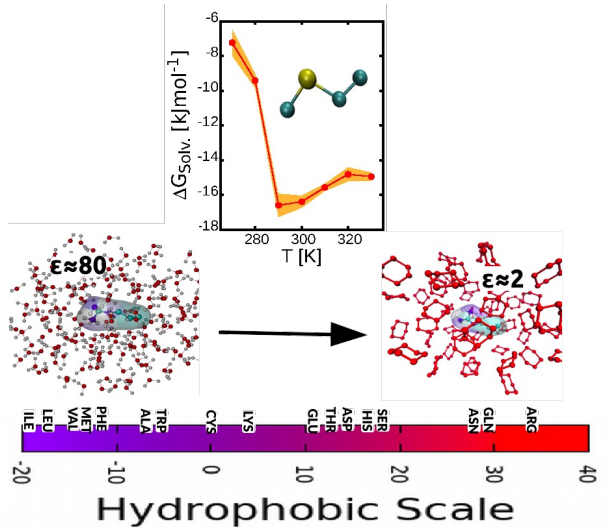


Liquid crystals



$$N \rightarrow N_S^* \rightarrow Sm_{A,S}^* \rightarrow Sm_{B,p}$$

Solvation free energies



Ca' Foscari University of Venice

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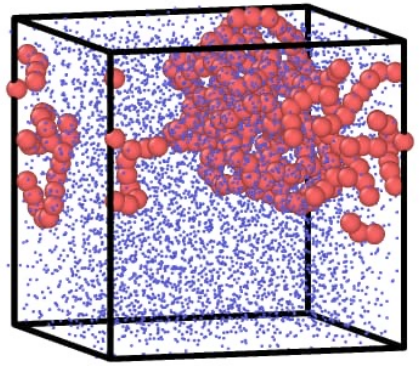
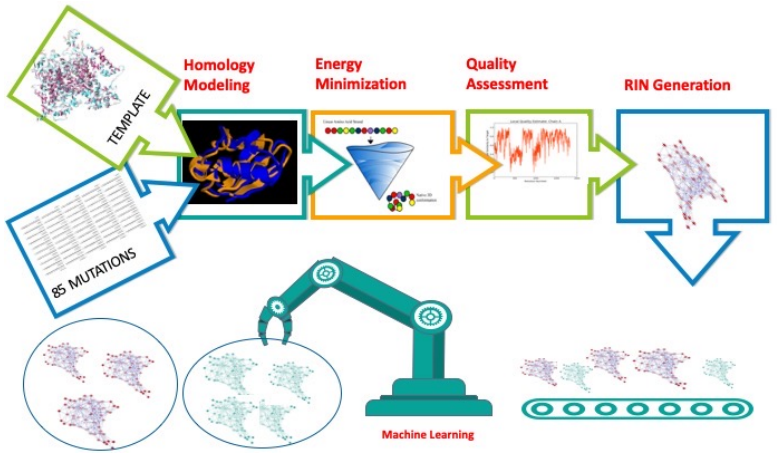
Our Lab

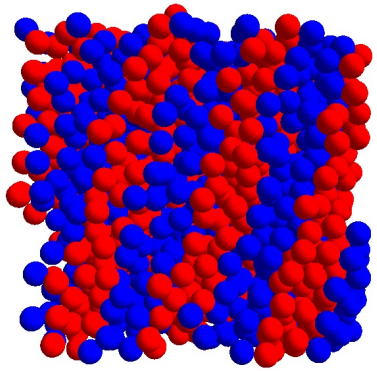
Polymers



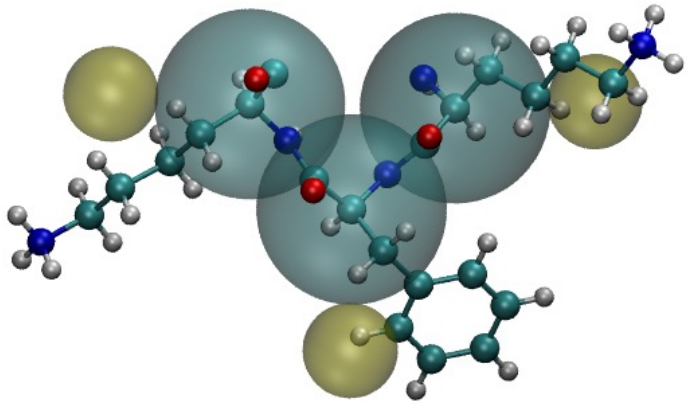
AI and Membrane Proteins



Colloids and patchy colloids



CG models for proteins



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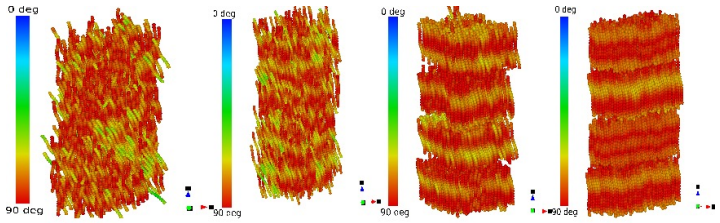
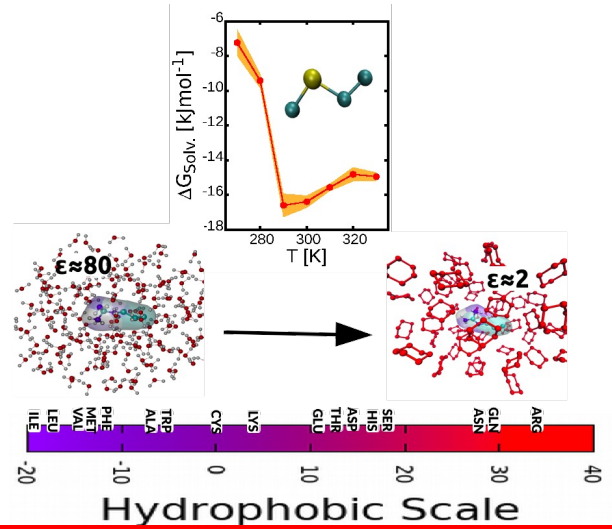


$$N \rightarrow N_S^* \rightarrow Sm_{A,S}^* \rightarrow Sm_{B,p}$$

Solvation free energies



Ca' Foscari University of Venice

Can Life exist without water?

www.unive.it

While water is an essential ingredient for life as we know it on Earth, there are some theories that suggest that life might be possible without water under certain conditions. However, no such life form has been discovered yet, and water remains the primary requirement for life as we know it.

Water plays a vital role in many of the chemical reactions that occur in living organisms, as well as providing a medium for the transport of nutrients and waste products. It is also a universal solvent, which means that it can dissolve many substances necessary for life.

That being said, there are some extremophile organisms on Earth that are able to survive in environments that are hostile to most life forms, such as in hot springs, deep-sea hydrothermal vents, or acidic environments. These organisms have adapted to these extreme conditions and have developed unique biochemical mechanisms that allow them to survive in the absence of water or with minimal amounts of water.

However, it is important to note that the search for life beyond Earth is based on our understanding of life as we know it on Earth, and the discovery of life forms that do not require water would require a rethinking of our definition of life and the conditions necessary for its existence.

NASA Report 2015

- Nearly 200 pages
- Water is mentioned 87 times

The origin and early evolution of life is another exciting key focus of astrobiology research. There are three components of these research efforts which include (1) understanding the sources of the organic building blocks of life and how they react to form the canonical macromolecules of life including nucleic acids, proteins, and lipid membranes; (2) taking advantage of advancements in molecular biology and biochemistry to better understand the diversity and evolutionary history of extant microbes as a window into better understanding the physiologies, including metabolisms, of the earliest organisms; and (3) merging the results from (1) and (2) to better constrain the environmental conditions that can spawn life. Astrobiology is also committed to understanding the

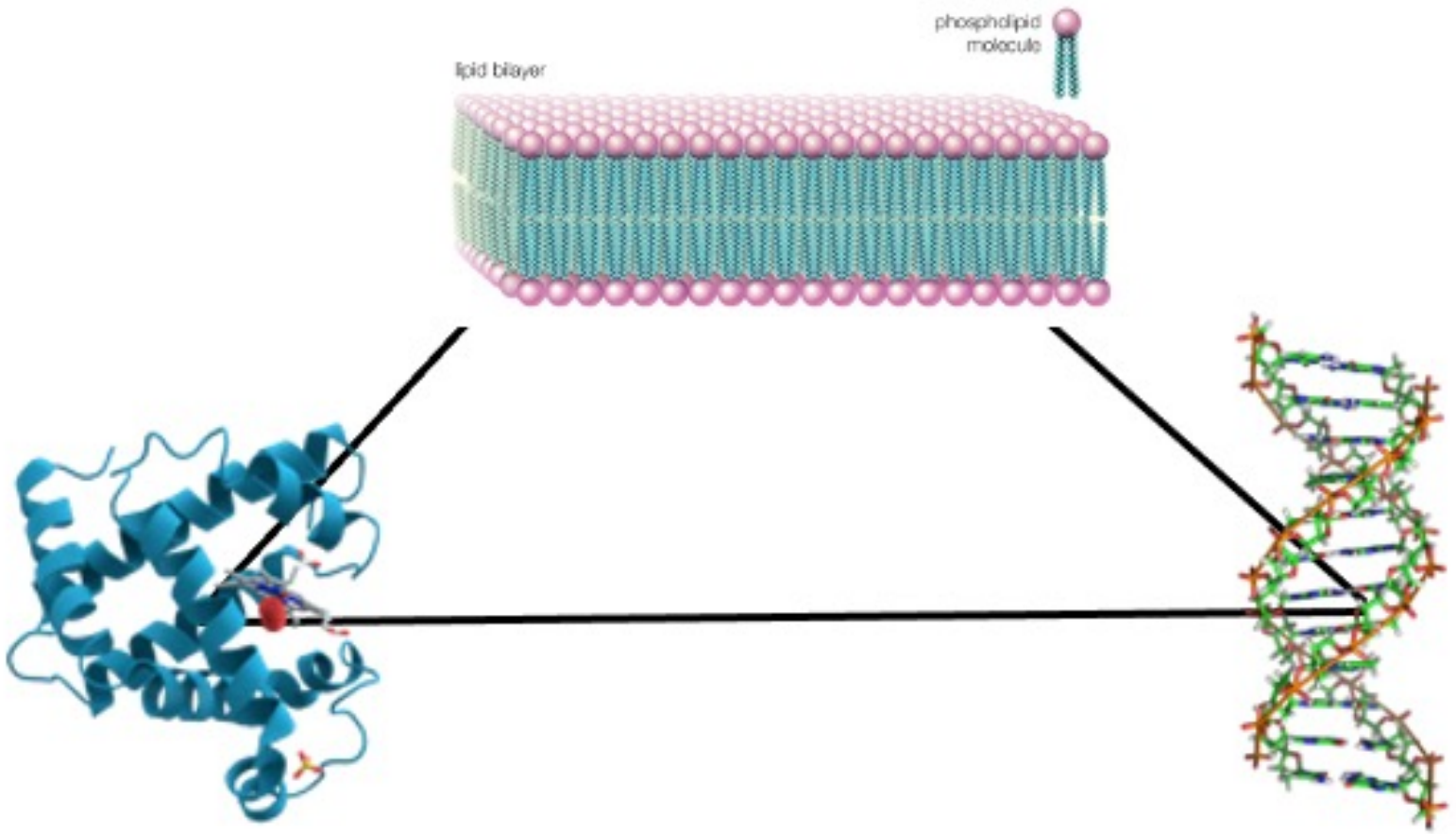
NASA Report 2015

determined the chemical makeup of the plumes, and amassed increasingly compelling evidence for a subsurface ocean there. Analysis of Titan's electric field recorded by the *Huygens* probe during its descent indicates that this moon likely has a salty subsurface sea, covered by an ice crust that is several tens of kilometers thick. Astrobiologists are intently studying the ever-present haze on Titan as an analog for the prebiotic organic chemical environment of early Earth, and have recently reported evidence for photochemical activity in Titan's lower atmosphere. *Cassini* observations have helped to better understand Titan's surface lakes of liquid ethane, methane, and propane, and laboratory simulations are being used to gain insight into these environments. Observations of Saturn's moon Dione indicate an active surface, with particles streaming off its surface and fractures in its ice similar to those seen on Enceladus. Scientists now think this moon may harbor a liquid water or slush layer underneath an outer icy shell.

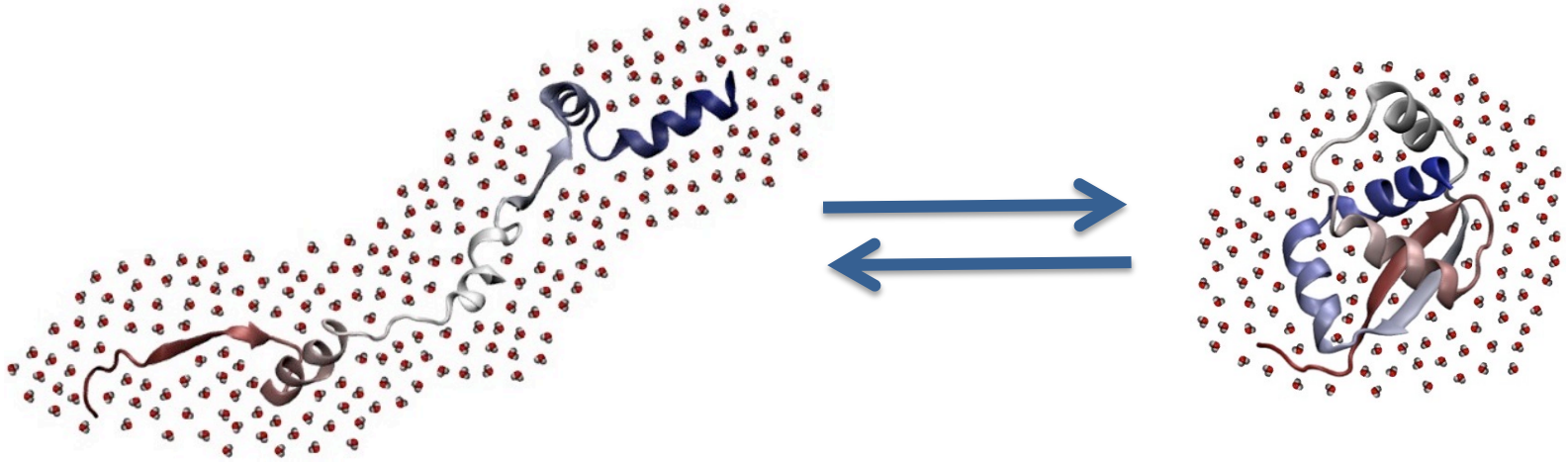
NASA Report 2015

Conceivably, some of our most fundamental concepts of life might still be too Earth-centric to capture the full diversity of life elsewhere. An alien biochemistry might not have the same chemistry exhibited in Earth-based life; for example, it might not have molecular backbones composed primarily of reduced carbon atoms. Solvents other than water might be capable of supporting an alien biochemistry. Some of the specific features we look for, such as the by-products of life's energy-obtaining strategies, may be different elsewhere. Any of these possibilities could expand the diversity of environments and planets on which life could exist and, therefore, modify the array of techniques we would utilize to search for life on those worlds.

THE TRIANGLE OF LIFE



The Hydrophobic Effect



[CONTRIBUTION FROM THE DEPARTMENT OF BIOCHEMISTRY, DUKE UNIVERSITY, MEDICAL CENTER, DURHAM, NORTH CAROLINA]

Contribution of Hydrophobic Interactions to the Stability of the Globular Conformation of Proteins

BY CHARLES TANFORD

RECEIVED APRIL 9, 1962

Ca' Foscari University of Venice

WATER!

www.unive.it

30 March
2022 / h 16:00

Auditorium
Danilo Mainardi

Campus Scientifico (Edificio ALFA)
Via Torino 155 - Venezia Mestre

Programme

› **16:00** Introduction

Achille Giacometti
ECLT Director
Ca' Foscari University of Venice

Francesca Tarocco
NICHE Director
Ca' Foscari University of Venice

› **16:15** Film screening

› **17:15** Discussion

Discussants

Anders Nilsson
Stockholm University
Stanford University

Francesco Sciortino
University of Rome "La Sapienza"

Mikael Agaton Director

WATER - The strangest liquid

AGATON FILM production
Mikael Agaton, Sweden, 2021 / 58'

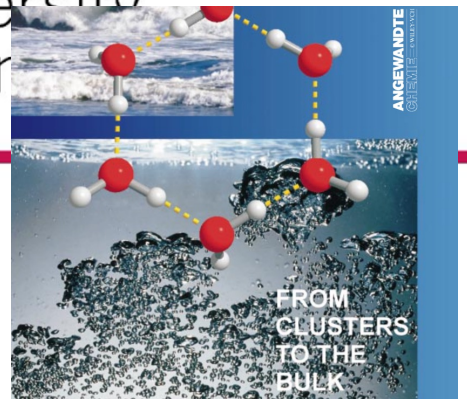
This documentary reveals stunning and groundbreaking discoveries about the most vital of substances, the one that constitutes most of ourselves: **water**. In this film the Swedish professor in physics at Stanford and Stockholm **Anders Nilsson** and his team of dedicated researchers enters the world of molecules and atoms under extreme conditions, and insist on designing and pursuing an experiment that nobody has considered possible. We follow their scientific journey from the hypothesis of two liquids from **Prof. Francesco Sciortino** towards the ultimate answer to why we are here at all: **why life can exist on the planet**.

More Info

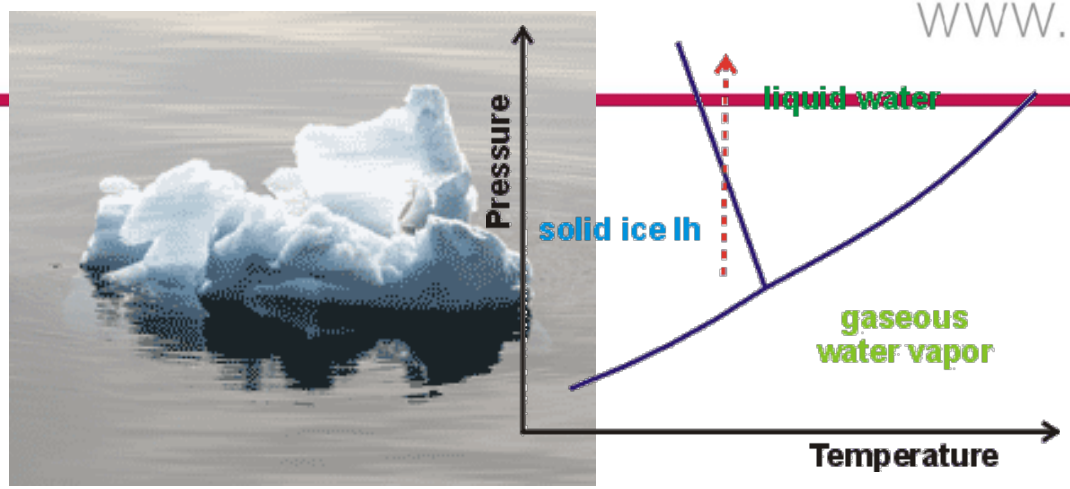
Registration is required, please contact **niche@unive.it** to receive registration form or zoom link. A valid Green Pass certificate is mandatory to access the venue.

www.unive.it/data/agenda/25/57742

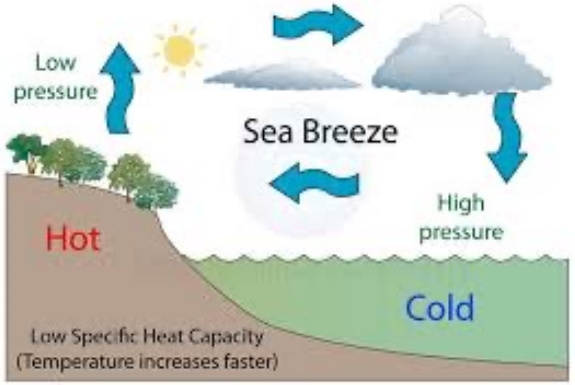
Water: what is so special about it?



- Water expands on freezing



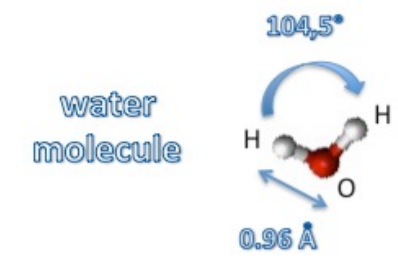
- High heat capacity

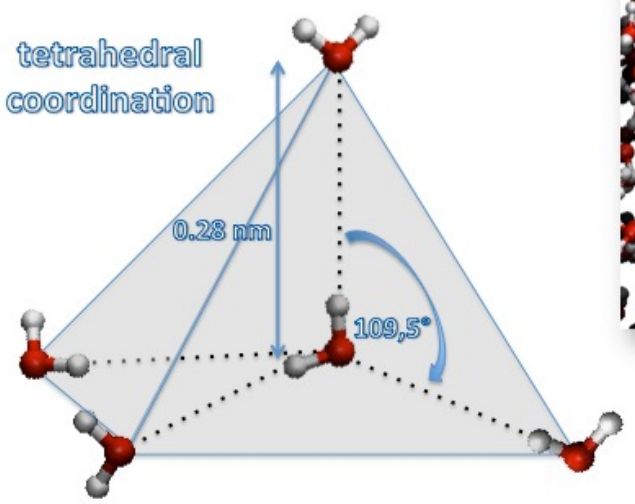


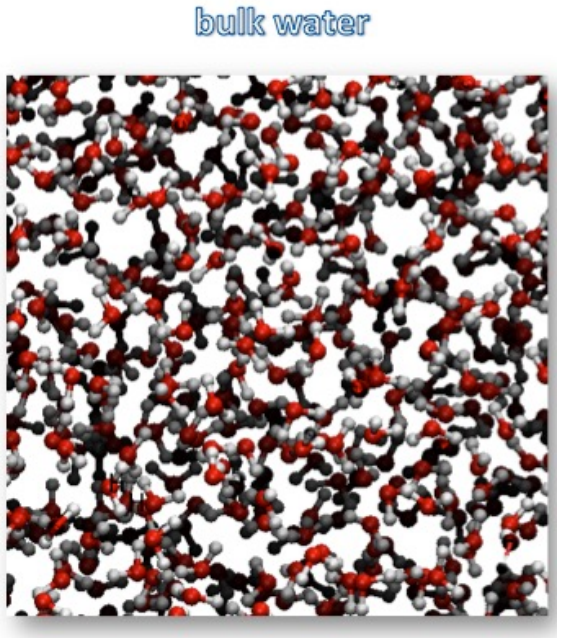
- High surface tension

….

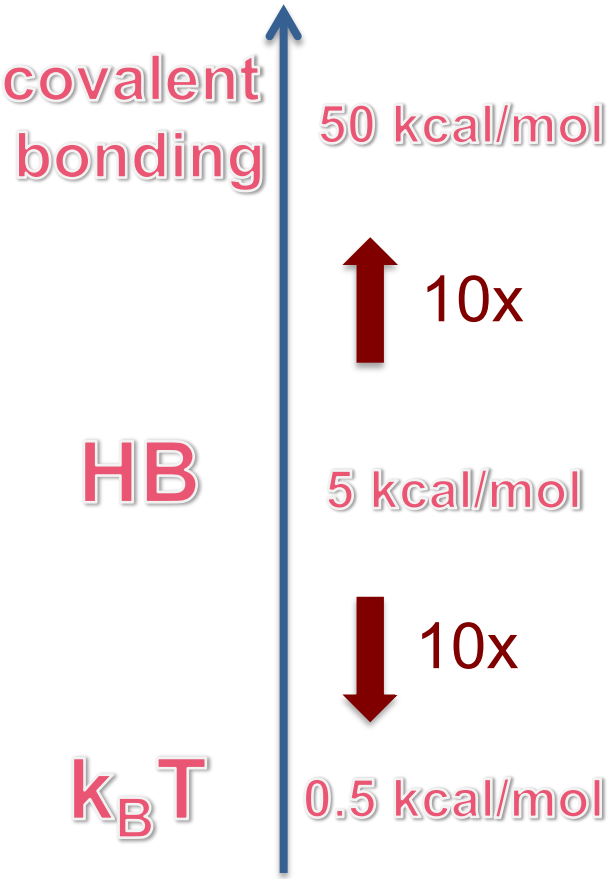
Water: what is so special about it?







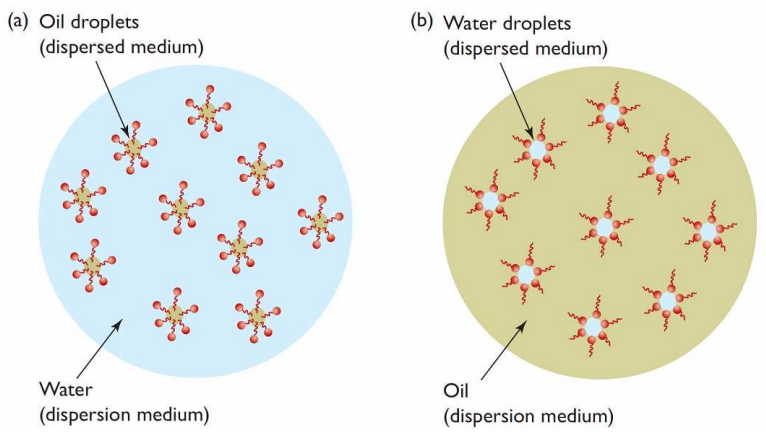
ε_r=80



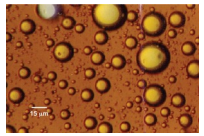
Symmetry polar-non polar?

Polar fluids water

Non Polar fluids oil



Surfactant



Ca' Foscari University of Ve

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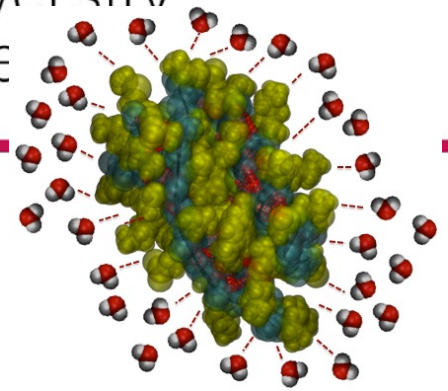
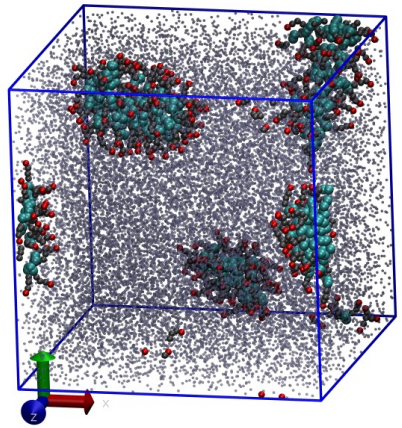
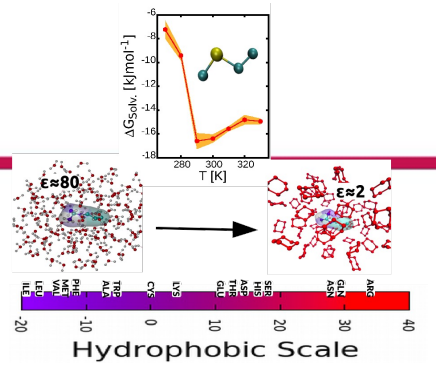
3 Stories



1: Approximate method for solvation free energy



2: Polarity-inverted Surfactants in non-polar solvents



#3 Solvation free energy of small peptides in non-polar solvents

Emanuele Petretto
Now @University of Friburg

Manuel Carrer
Now @University of Oslo

Cedrix Dongmo
Ca' Foscari University of Venice/University of Rome 2

Tatjana Skrbic
University of Oregon/ Ca' Foscari University of Venice

Amino acid structures

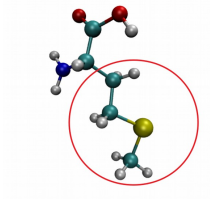
Ca' Foscari University of

www.unive.it

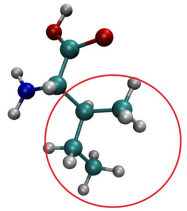
HYDROPHOBIC

Aliphatic non-polar

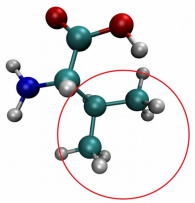
METHIONINE
MET/M



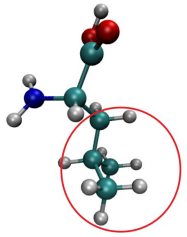
ISOLEUCINE
ILE/I



VALINE
VAL/V

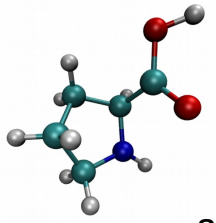


LEUCINE
LEU/L

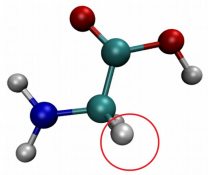


Special cases

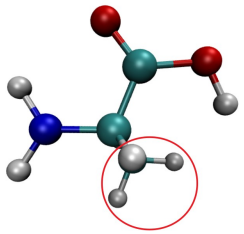
PROLINE
PRO/P



GLYCINE
GLY/G

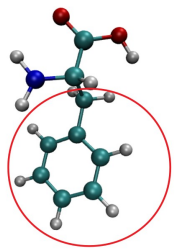


ALANINE
ALA/A

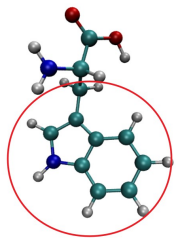


Aromatic non-polar

PHENYLALANINE
PHE/F



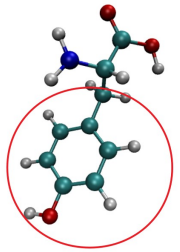
TRYPTOPHAN
TPR/W



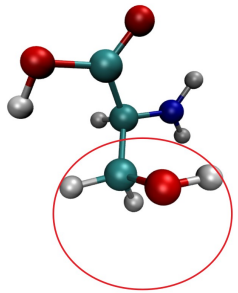
POLAR

Uncharged

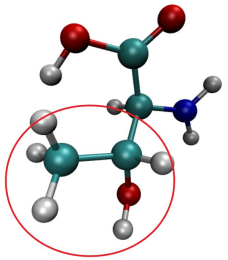
TYROSINE
TYR/Y



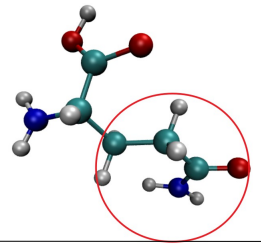
SERINE
SER/S



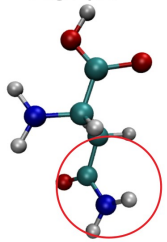
THREONINE
THR/T



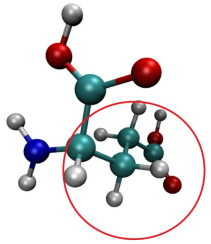
GLUTAMINE
GLN/Q



ASPARAGINE
ASP/N



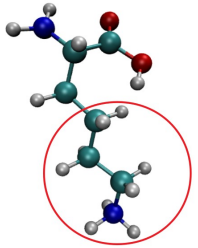
GLUTAMIC ACID
GLU/E

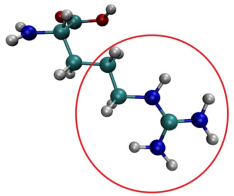


Positively charged

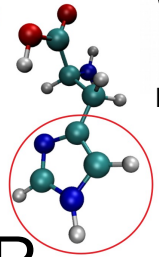
ARGININE
ARG/R

LYSINE
LYS/K

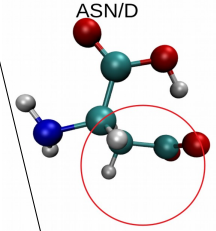




HISTIDINE
HIS/H

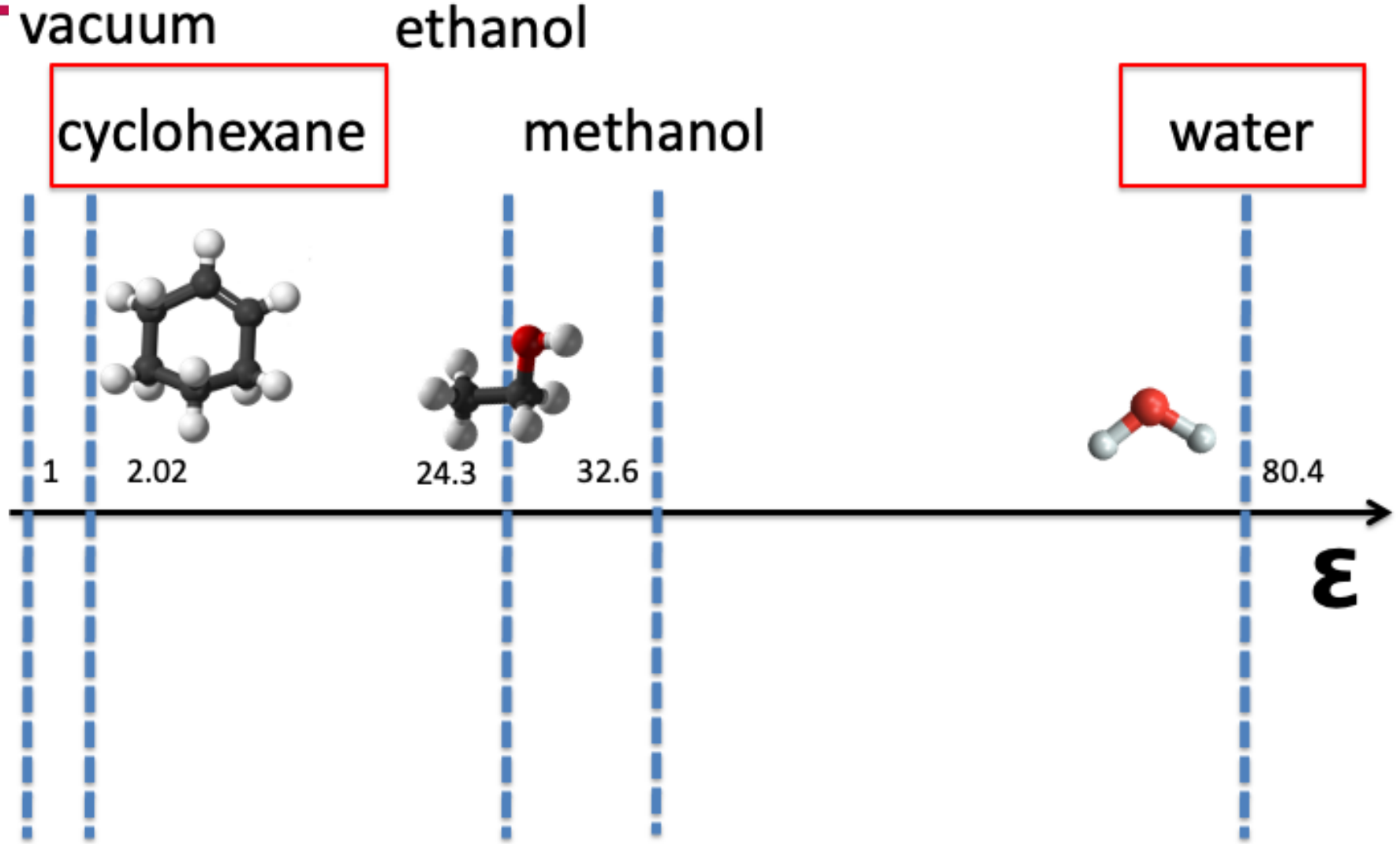


ASPARTIC ACID
ASN/D



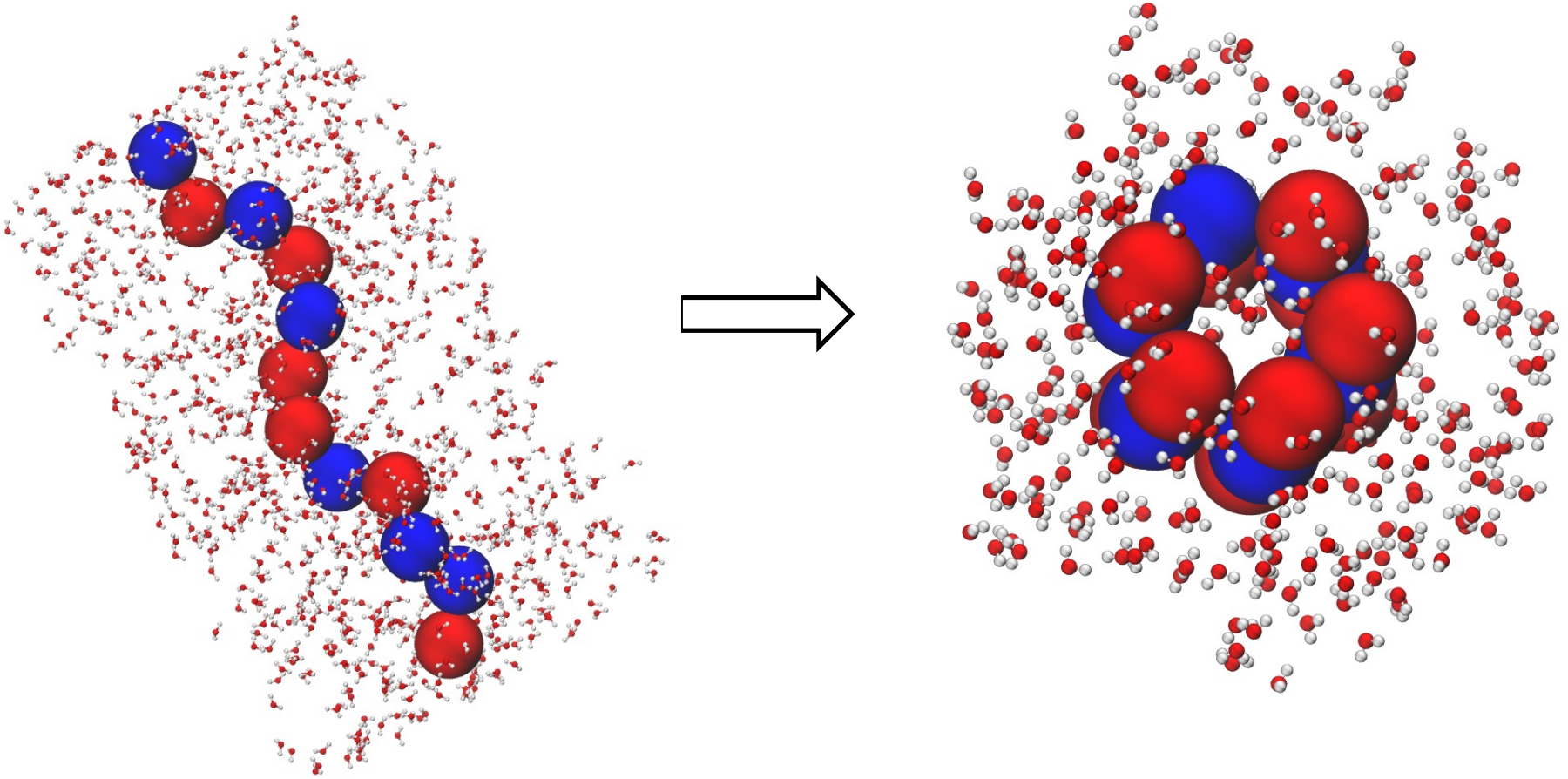
Negatively charged

Solvent polarity scale



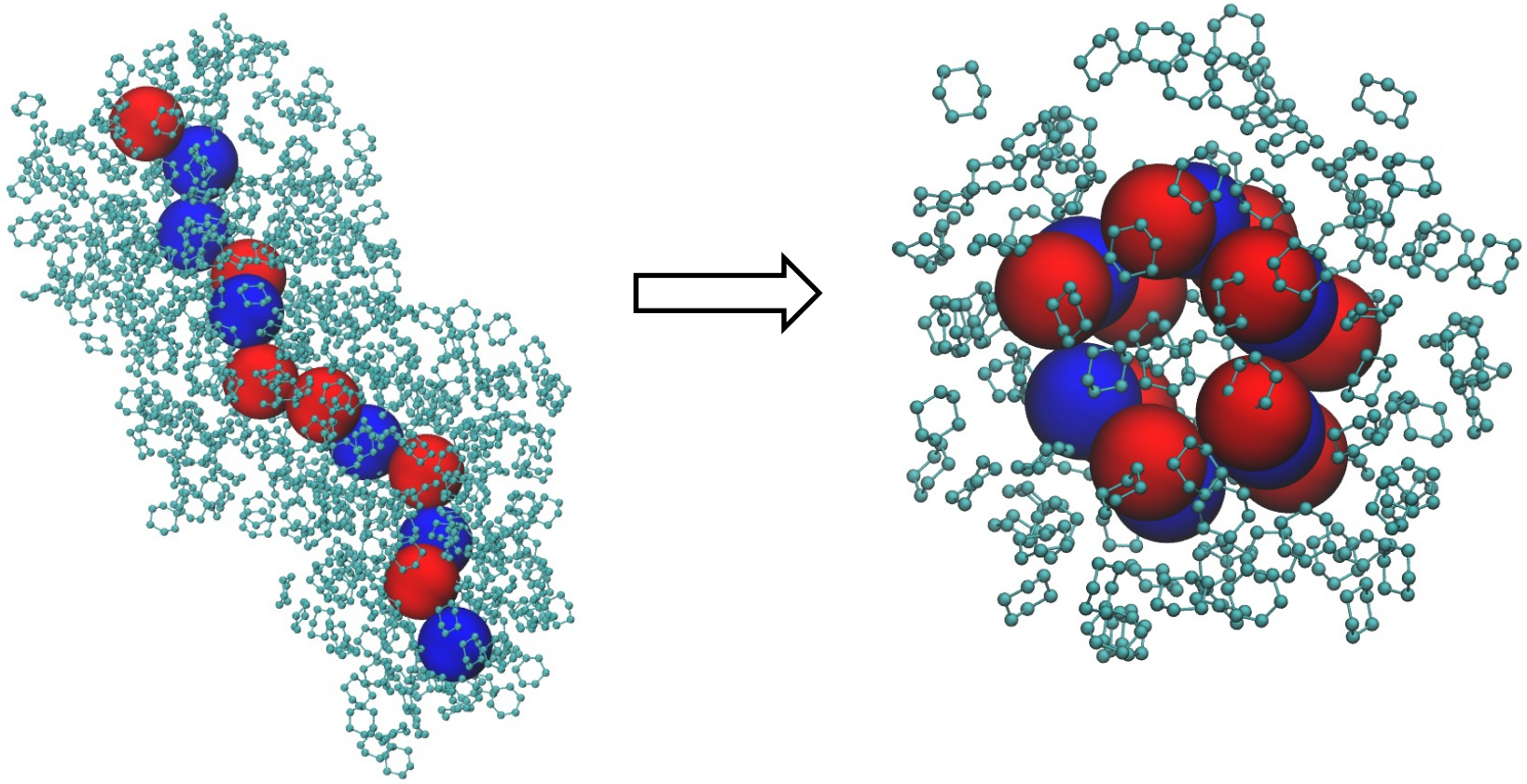
The hydrophobic effect

P H

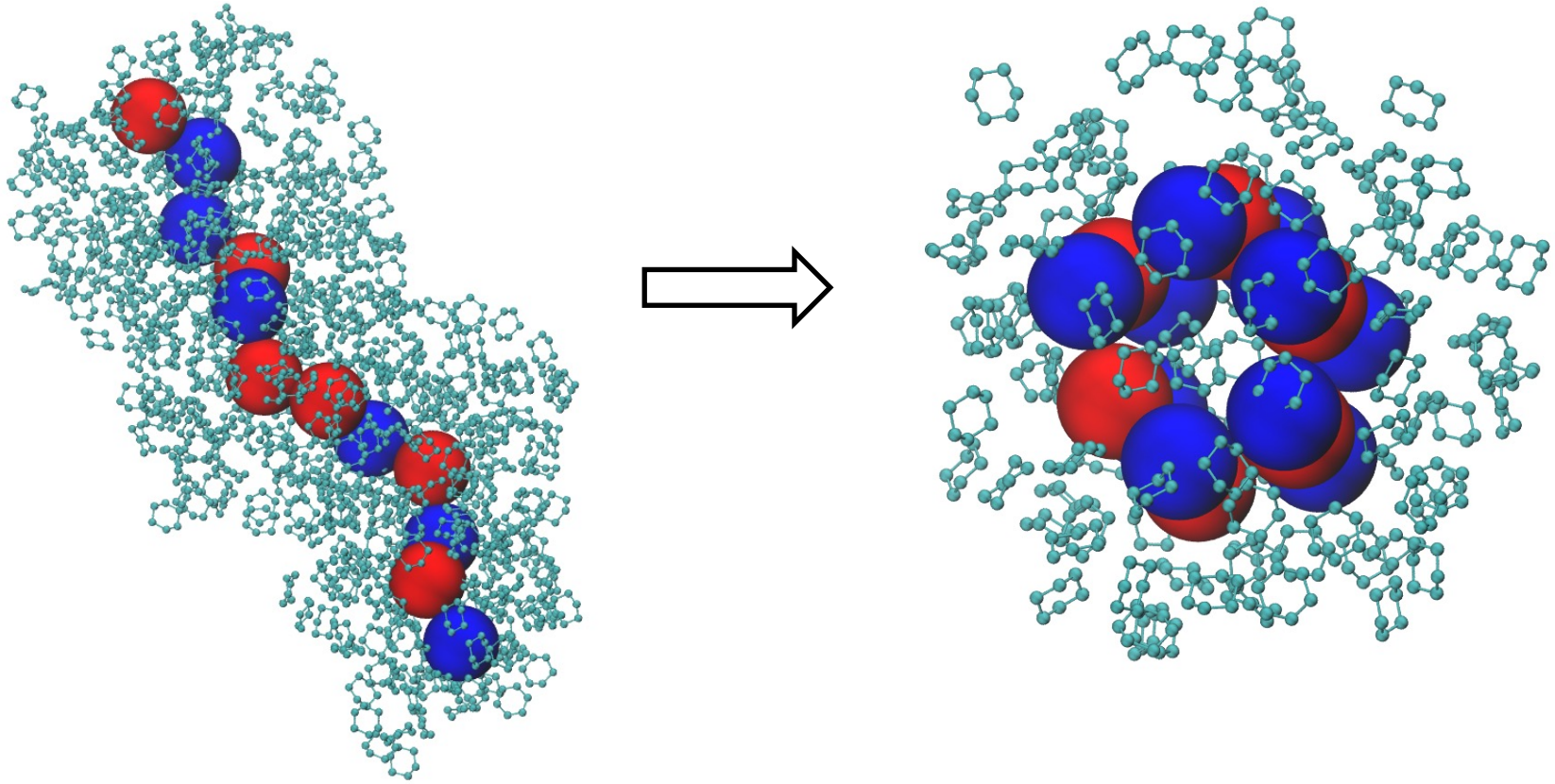


P H

Same fold?



Like dissolves like?



No definitive Experimental evidence

insight review articles

Improving enzymes by using them in organic solvents

Alexander M. Klibanov

Department of Chemistry, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139, USA (e-r

THE ROYAL SOCIETY

J. Am. Chem. Soc. **1993,** *115,* 6529–6537

Protein Dynamics and Solvation in Aqueous and Nonaqueous Environments

David S. Hartsough and Kenneth M. Merz, Jr.*

Contribution from the Department of Chemistry, 152 Davey Laboratory, Pennsylvania State University, University Park, Pennsylvania 16802

Protein structure, stability and solubility in water and other solvents

C. Nick Pace*, Saul Treviño, Erode Prabhakaran and J. Martin Scholtz

Department of Medical Biochemistry and Genetics, Department of Biochemistry and Biophysics and Center for Advanced Biomolecular Research, Texas A&M University, College Station, TX 77843, USA

 Biophysical Journal Volume 84 March 2003 1628–1641

Protein Structure and Dynamics in Nonaqueous Solvents: Insights from Molecular Dynamics Simulation Studies

Cláudio M. Soares, Vitor H. Teixeira, and António M. Baptista

Instituto de Tecnologia Química e Biológica, Universidade Nova de Lisboa, Av. da República, Apartado 127, 2781-901 Oeiras, Portugal

Ca' Foscari University of Venice

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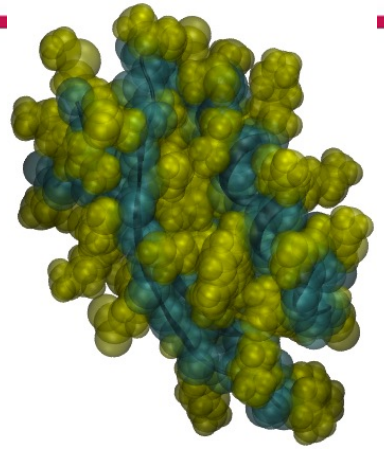
#1 Solvent polarity effects on protein stability

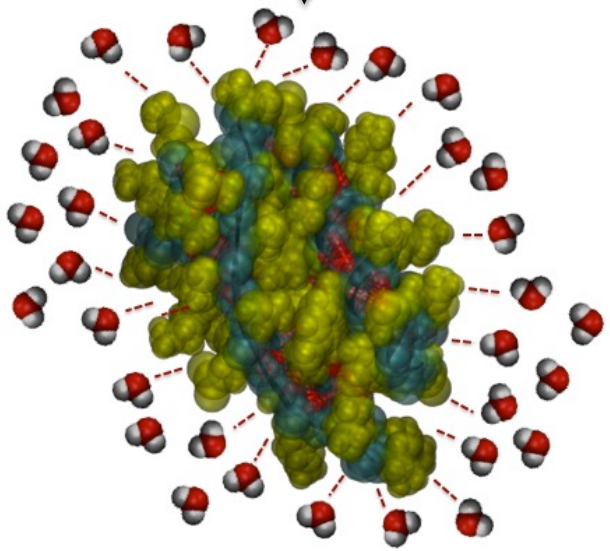
Masahiro Kinoshota University of Kyoto

Emanuele Petretto

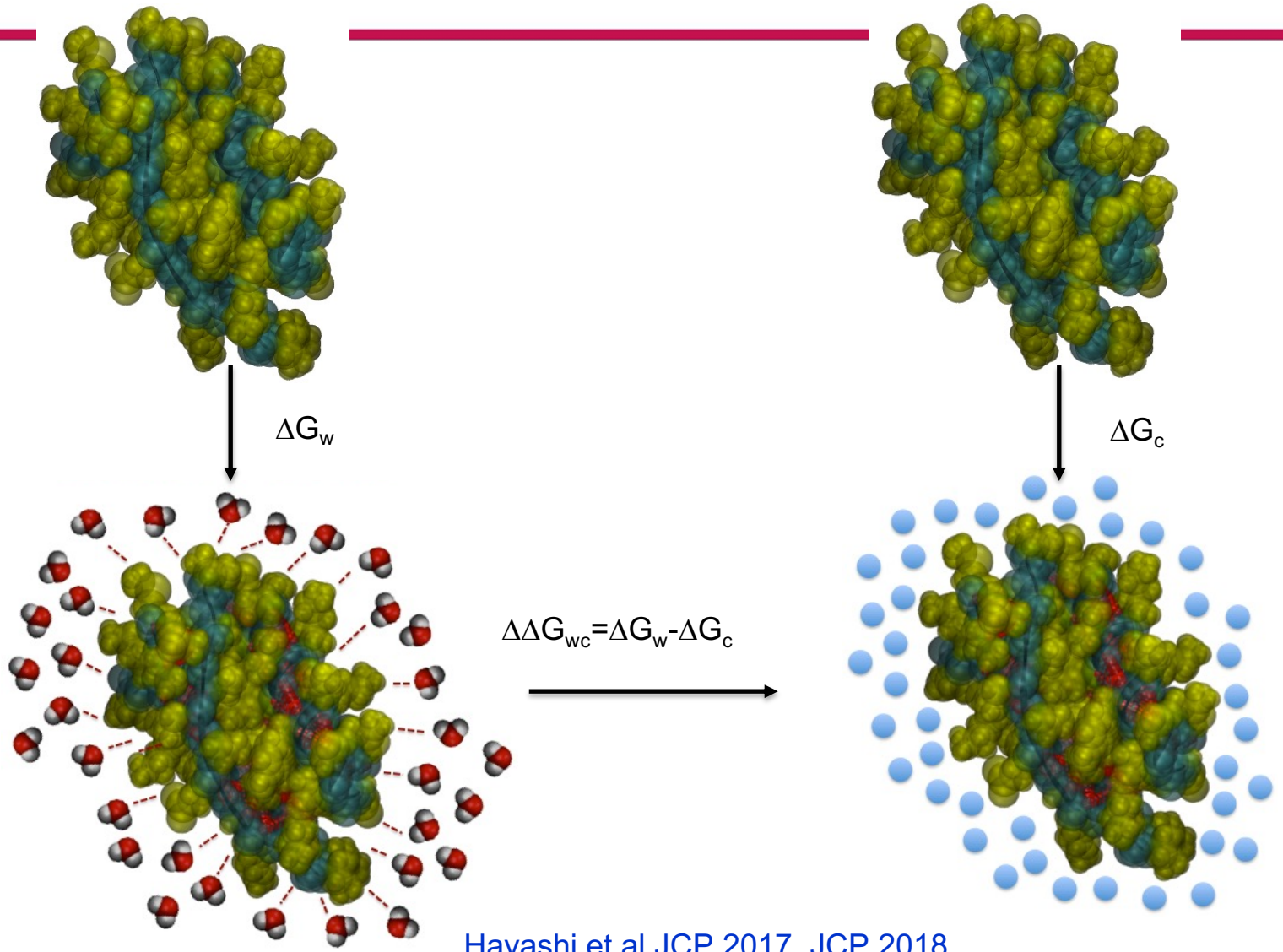
Now @University of Friburg



ΔG_w Solvation free energy



Thermodynamic cycle



Hayashi et al JCP 2017, JCP 2018

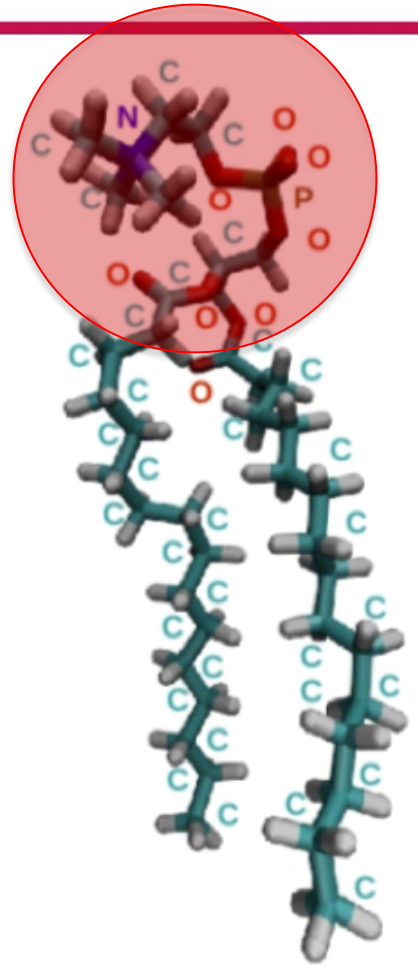
Ca' Foscari University of Venice

#2: Surfactants

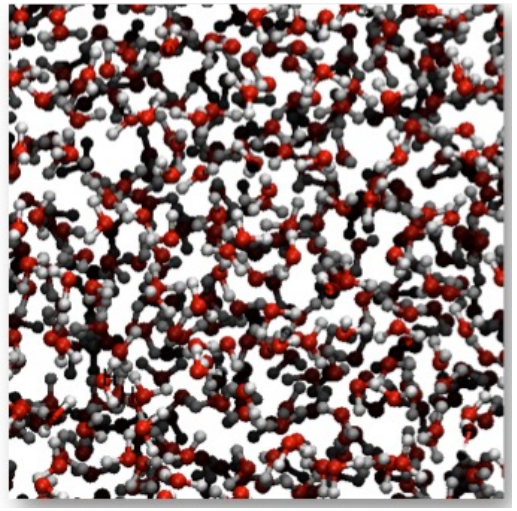
Manuel Carrer
Now @University of Oslo

www.unive.it

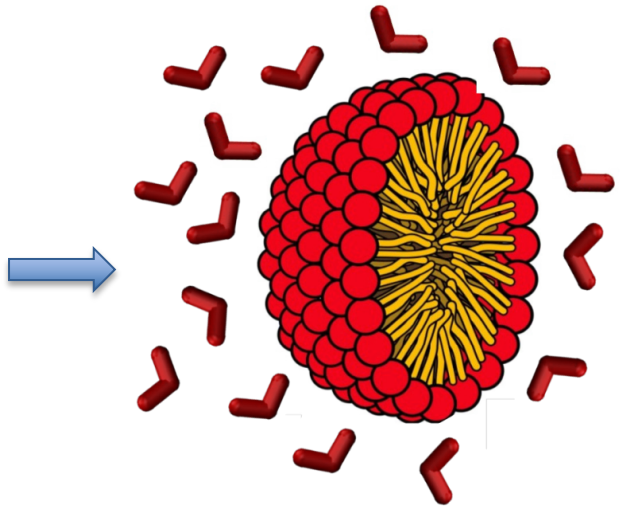
With Michele Cascella



DPPC (Dipalmitoylphosphatidylcholine)

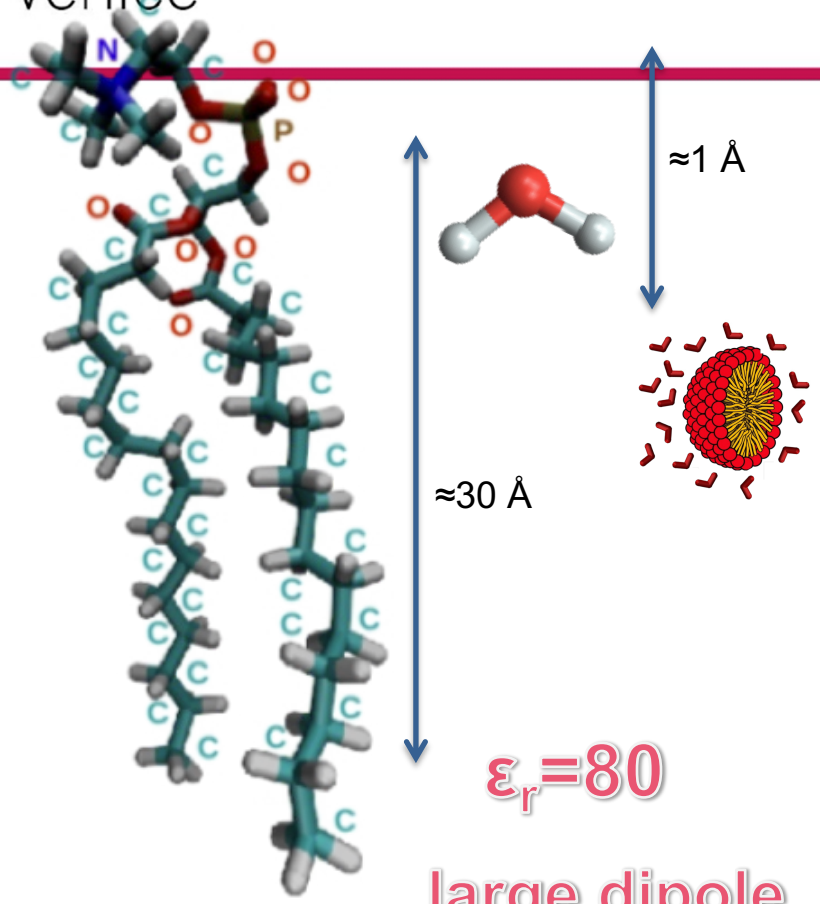


Water



Micelles

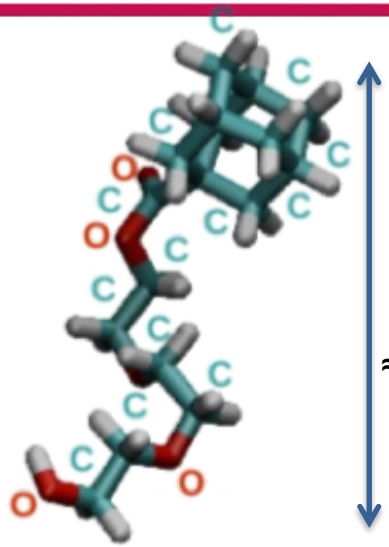
Length and energy scales



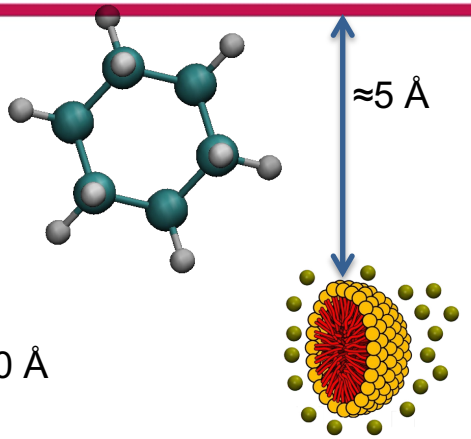
DPPC

ε_r=80

large dipole moment



ADOH

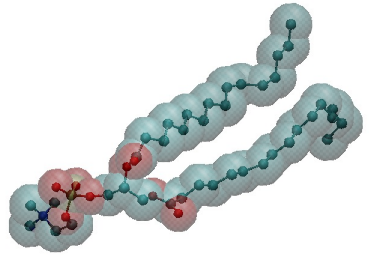


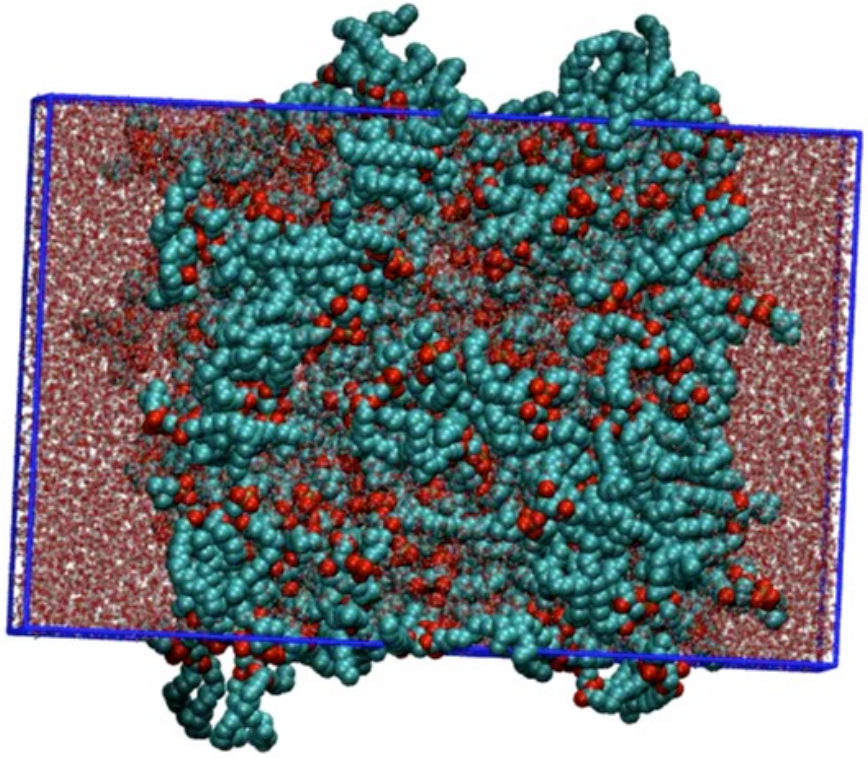
ε_r=2

no dipole moment
first non-zero moment is quadrupole

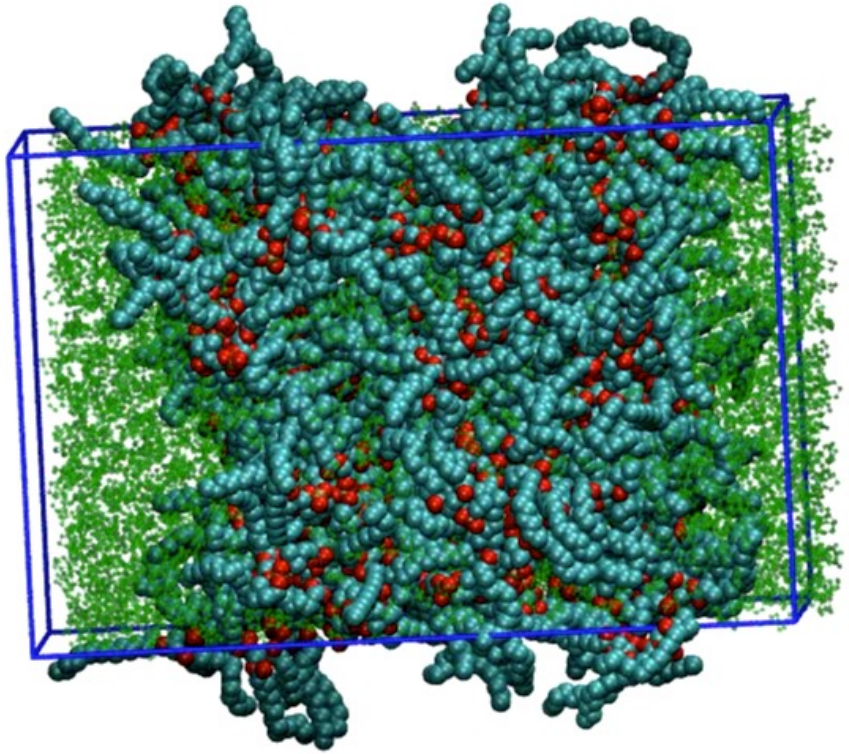
Conventional surfactants: DPPC

Skrbic et al unpublished





Water



CHEX

#3: Exact Solvation free energy of polypeptides

Ca' Foscari University of Venice

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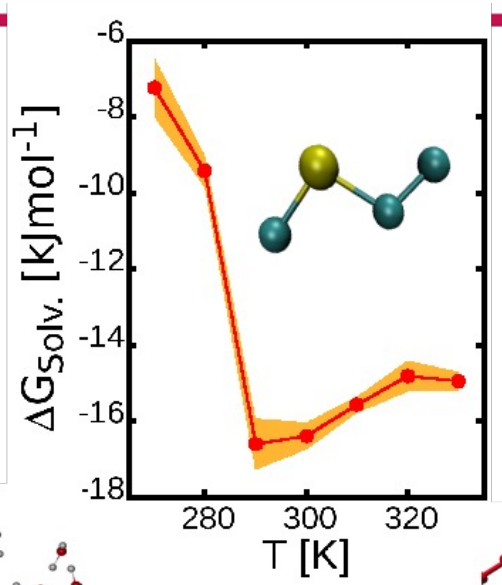
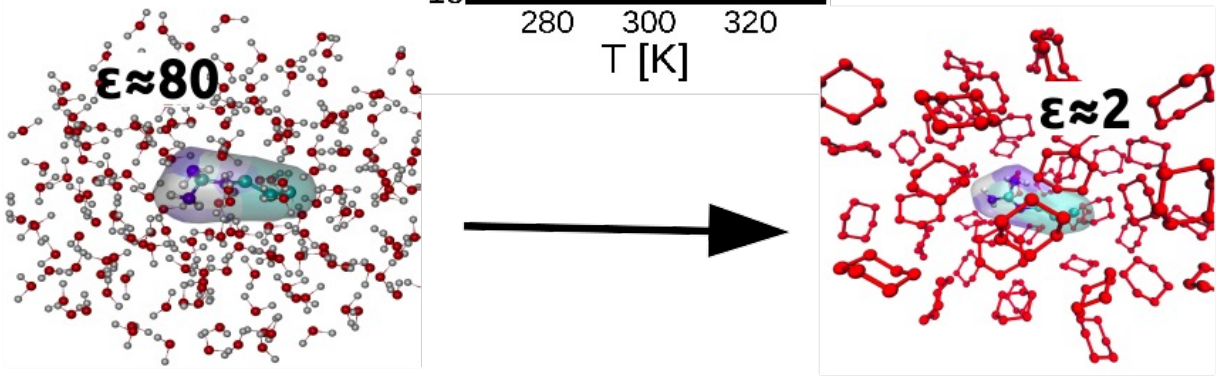


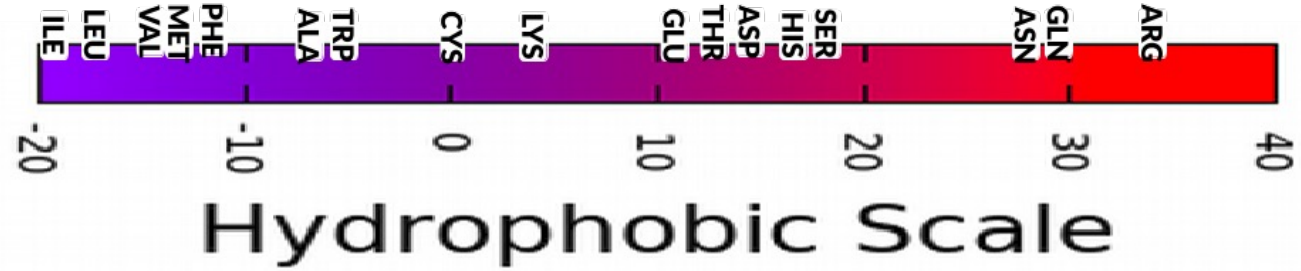
Dongmo et al PCCP 2020

Dongmo, Giacometti PCCP 2023



Cedrix Dongmo
Ca' Foscari
University of Venice

With Giuseppe Graziano



Ca' Foscari University of Venice

Data driven approach: November 2020!

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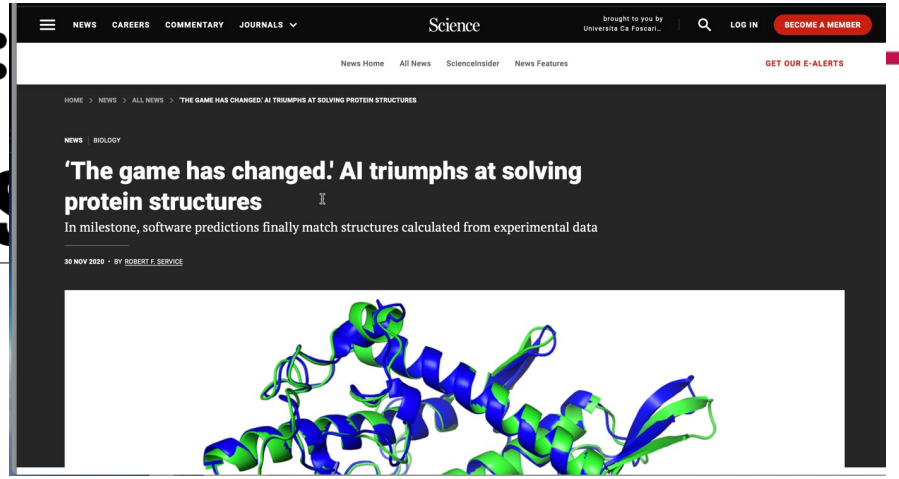
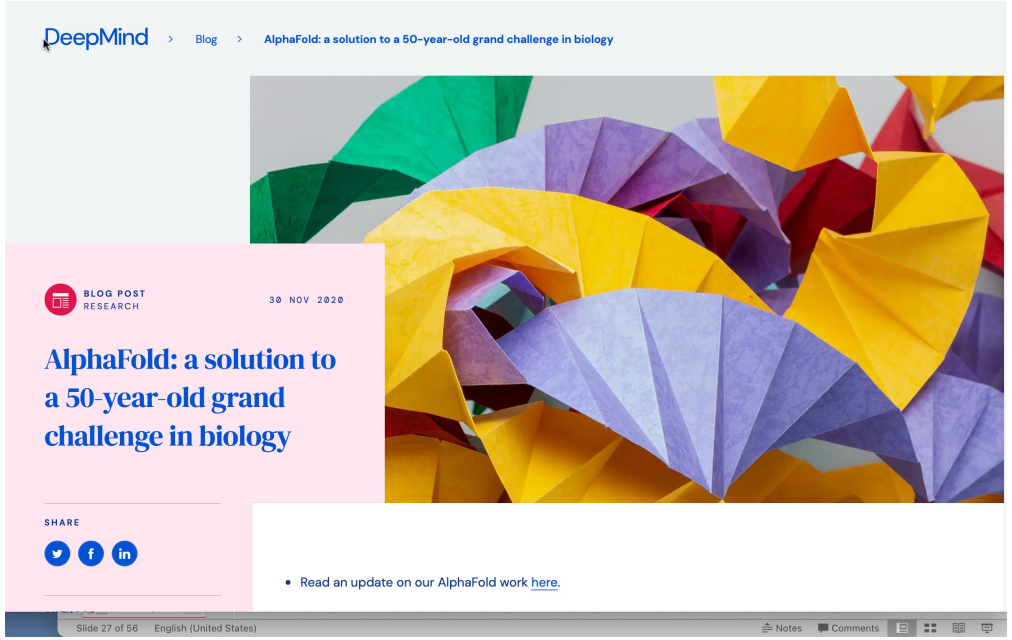
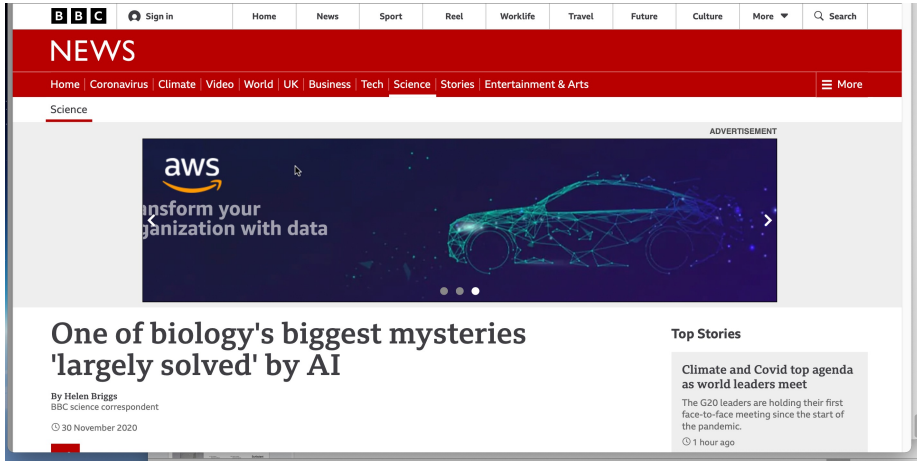
'IT WILL CHANGE EVERYTHING': AI MAKES GIGANTIC LEAP IN SOLVING PROTEIN STRUCTURES

DeepMind's program for determining the 3D shapes of proteins stands to transform biology, say scientists.



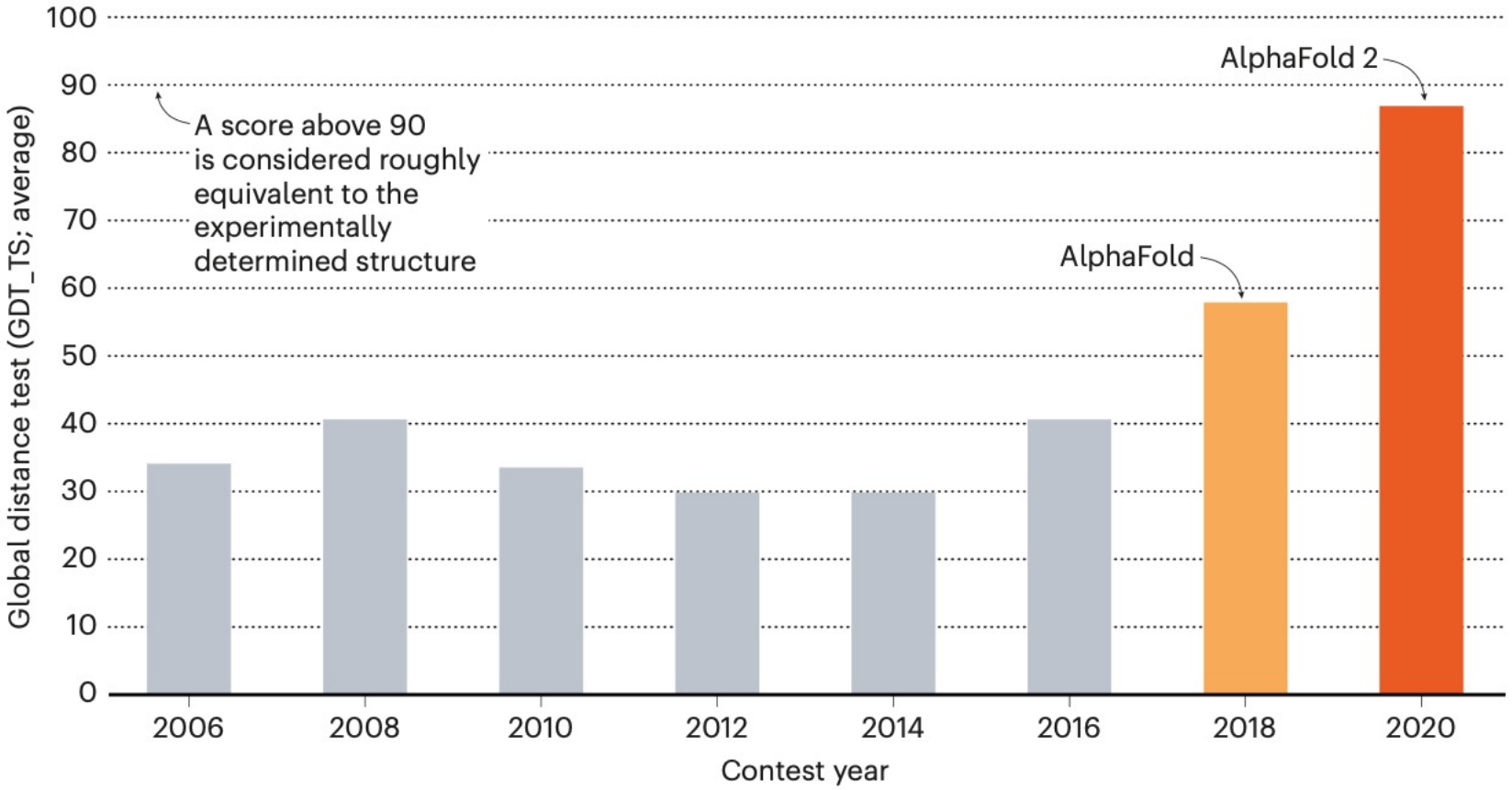




CASP14 2020

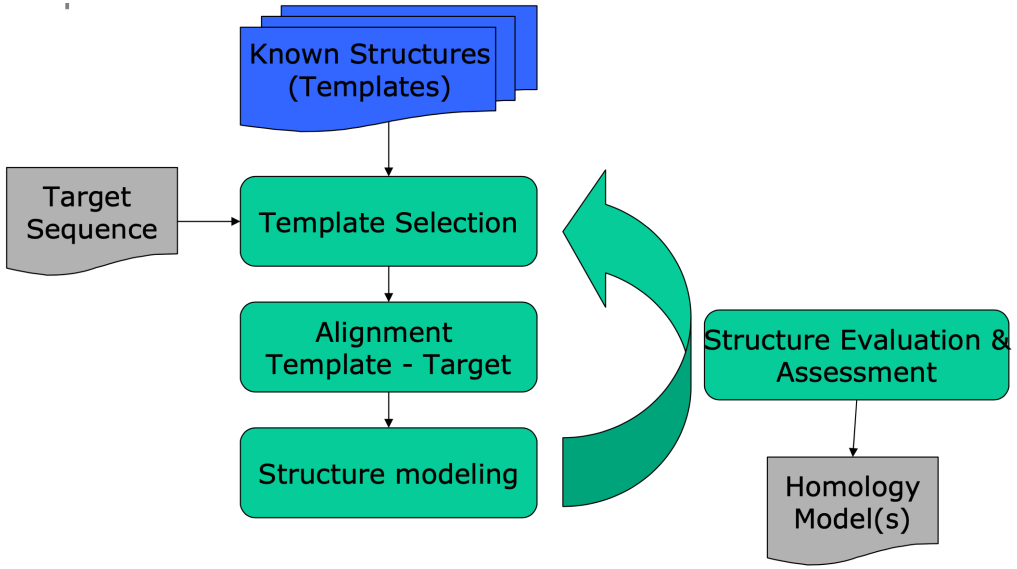
STRUCTURE SOLVER

DeepMind's AlphaFold 2 algorithm significantly outperformed other teams at the CASP14 protein-folding contest — and its previous version's performance at the last CASP.

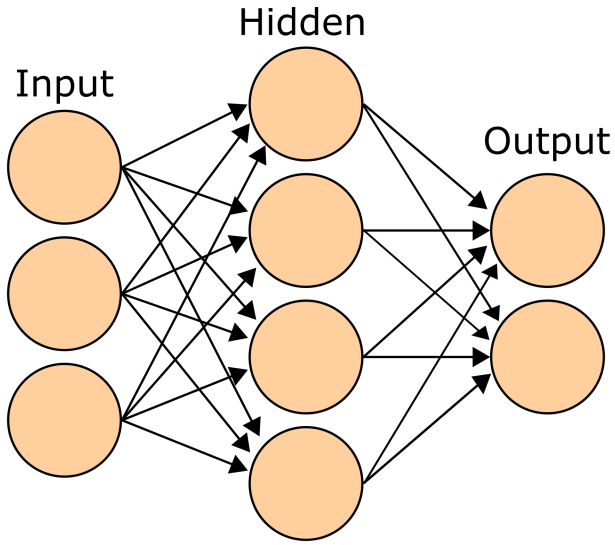


How was this achieved?

Homology modeling



Machine Learning (AI)



Google vs Baker's group

Article

Highly accurate protein structure prediction with AlphaFold

https://doi.org/10.1038/s41586-021-03819-2

Received: 11 May 2021

Accepted: 12 July 2021

Published online: 15 July 2021

Open access

Check for updates

John Jumper[1,4]✉, Richard Evans[1,4], Alexander Pritzel[1,4], Tim Green[1,4], Michael Figurnov[1,4], Olaf Ronneberger[1,4], Kathryn Tunyasuvunakool[1,4], Russ Bates[1,4], Augustin Žídek[1,4], Anna Potapenko[1,4], Alex Bridgland[1,4], Clemens Meyer[1,4], Simon A. A. Kohl[1,4], Andrew J. Ballard[1,4], Andrew Cowie[1,4], Bernardino Romera-Paredes[1,4], Stanislav Nikolov[1,4], Rishub Jain[1,4], Jonas Adler[1], Trevor Back[1], Stig Petersen[1], David Reiman[1], Ellen Clancy[1], Michal Zielinski[1], Martin Steinegger[2,3], Michalina Pacholska[1], Tamas Berghammer[1], Sebastian Bodenstein[1], David Silver[1], Oriol Vinyals[1], Andrew W. Senior[1], Koray Kavukcuoglu[1], Pushmeet Kohli[1] & Demis Hassabis[1,4]✉

RESEARCH ARTICLE

Breakthrough of the year 2021

PROTEIN FOLDING

Accurate prediction of protein structures and interactions using a three-track neural network

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Data Driven Approach?

interactions with the planet increased in diversity, eventually developing into complex feedbacks. By studying this co-evolutionary past, we deepen our understanding of habitability and learn about significant branch points in the history of the habitability of Earth-like planets. Finally, studies of other planets—both real and hypothetical—inform and benefit from work on the intimate interactions between life and its physical environment. Observations of specific habitable environments in planets and moons in our Solar System can illuminate the properties of Earth that permitted life to flourish here, suggest the potential for life on other bodies in our Solar System, and provide a foundation to model rocky planets in other planetary systems. Furthermore, as we explore planets in and beyond our Solar System, we must develop the capacity to assess the habitability of these environments and to recognize and characterize signatures of life—from the microscopic to the planetary scale. These efforts to identify and characterize biosignatures are necessarily informed by close examination of Earth's past, present, and future.

The TEAM