Graph Theory for Molecular Dynamics Simulations

Prof. Marie-Pierre Gaigeot

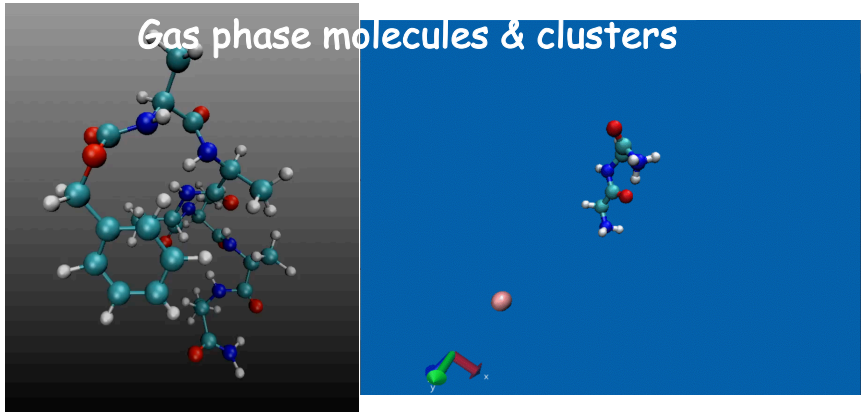
LAMBE Laboratoire Analyse et Modélisation
pour la Biologie et l'Environnement - UMR 8587 CNRS
Université d'Evry val d'Essonne - Paris France
Université Paris-Saclay - France

FRSC Fellow of the Royal Society of Chemistry
Overseas Fellow @ Churchill College Cambridge-UK
IUF Institut Universitaire de France

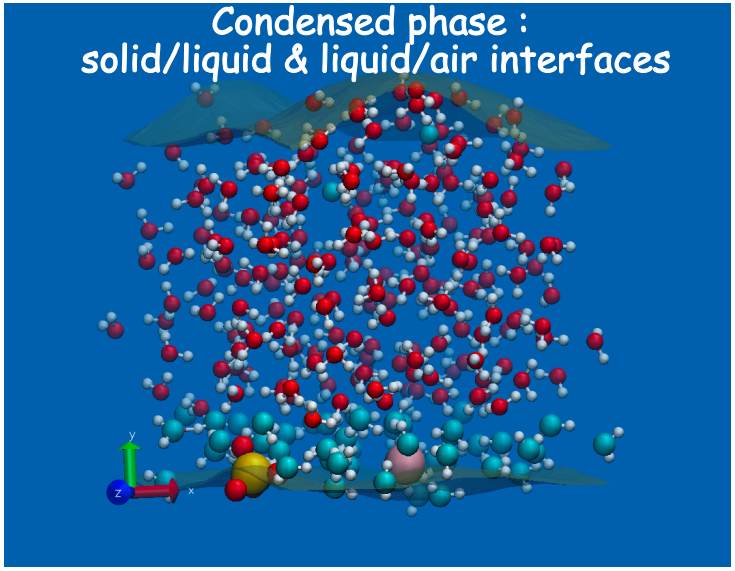
mgaigeot@univ-evry.fr
http://mpgaigeot-research.fr

Graph theory algorithms in MD simulations

Analyze trajectories with 2D-graphs



3D-structures over time, isomerization, HB dynamics, proton transfers, dynamics of fragmentation, fragments, pathways, …



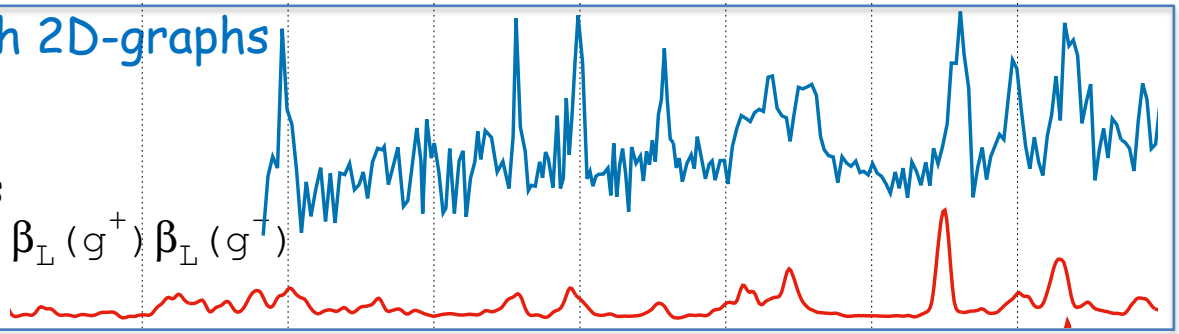
Structure of BIL, location of ions, H-Bond dynamics, …

Structures and Dynamics for the molecular interpretation of vibrational spectroscopies (IR, Raman, SFG), CID, heterogeneous catalysis, ….

Analyze vibrational spectra with 2D-graphs

Give the molecular assignment of the anharmonic modes in each peak → interpret experiments

Maps of vibrational motions



Graph theory + Game theory & Machine-/Deep-/Reinforcement Learning(s)

Coupling graphs, learning methods, game theory for high throughput 3D-structures discovery from spectroscopies : reverse discovery of 3D structures

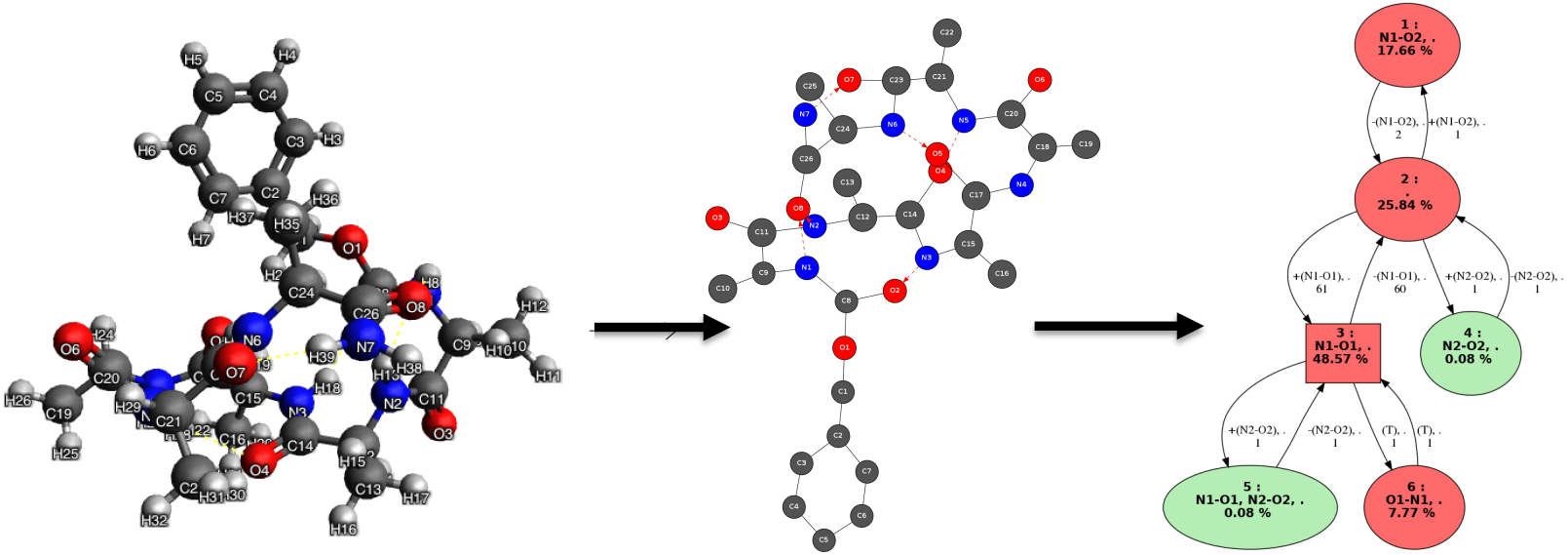
Graph theory and 3D-structures : 2D-Molecular Graphs

Graph theoric algorithms for the automatic recognition of molecular structures along MD simulations

Transferable algorithms

- ✓ Gas phase molecules and clusters (peptides, proteins, DNA, saccharides, …)
- ✓ Solids, Liquids
- ✓ Inhomogeneous interfaces : solid/liquid, liquid/air, ….

Recognition of changes in the structures in terms of H-Bonds, covalent bonds, electrostatic interactions (ion shells), organometallics, ….



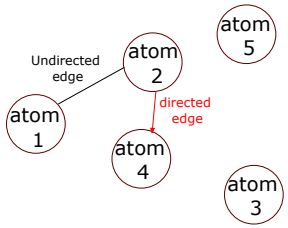
3D-conformation | 2D-Molecular Graph | Graph of transitions

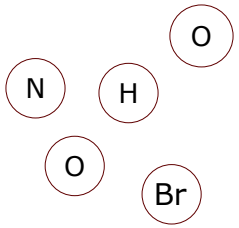
Bougueroua, Barth, Quessette, Spezia, Vial, Gaigeot, J. Chem. Phys. 2018

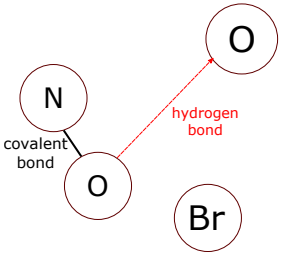
GaTewAY software

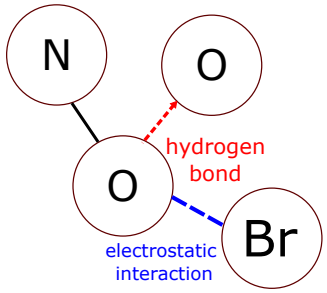
Graph theory and 3D-structures : 2D-Molecular Graphs

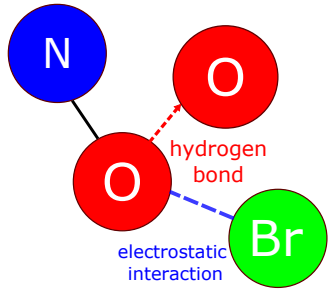
Graph theoric algorithms for the automatic recognition of molecular structures along MD simulations











A molecular conformation is a mixed graph $G(V,E_c,A_H,E_I,E_O)$

directed edges (DE) & undirected edges (UDE)

V: vertices made of the molecular atoms (no H)

Ec: UDE made of covalent bonds

A_H: DE made of H-Bonds

E_I: UDE made of electrostatic interactions (ions)

E_O: UDE made of 'organometallic interactions'

Vertices are colored

Key algorithms : isomorphism

Identify :

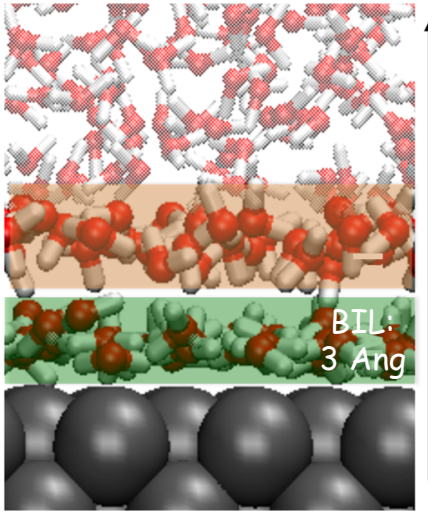
- conformers that are explored over time + life-times
- conformational changes over time, isomerization, proton transfers, …
- transitions between structures, quantification of occurrences, A→B vs B→A, …
- connected components, fragments, (repeated) motifs, in the structure + time-evolution

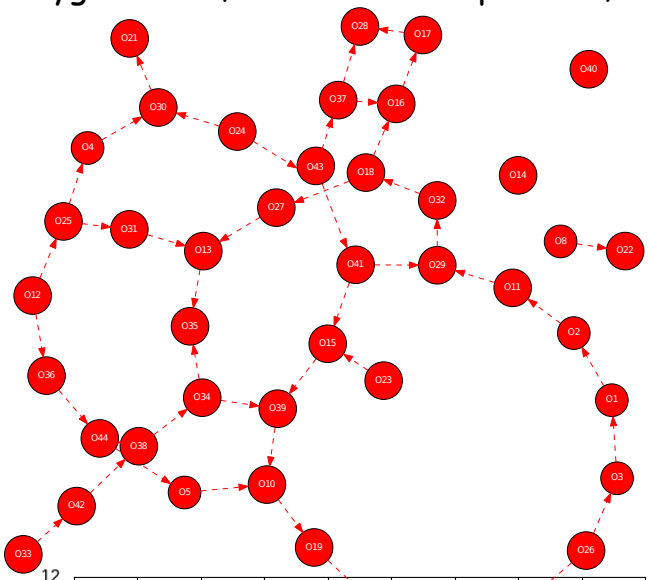
Bougueroua, Barth, Quessette, Spezia, Vial, Gaigeot, J. Chem. Phys. 2018

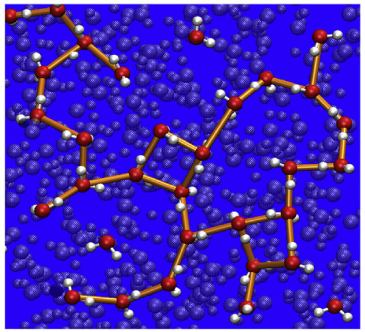
Illustration on condensed matter : the 2D-MolGraph directly shows the collective arrangement of water at hydrophobic interfaces

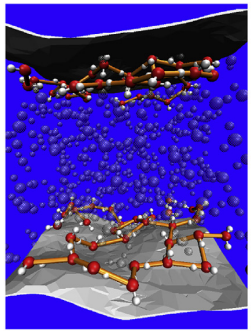
BIL-water : 2D-MolGraph → 2D-Hbond-Network made of adjacent 2D-polygons

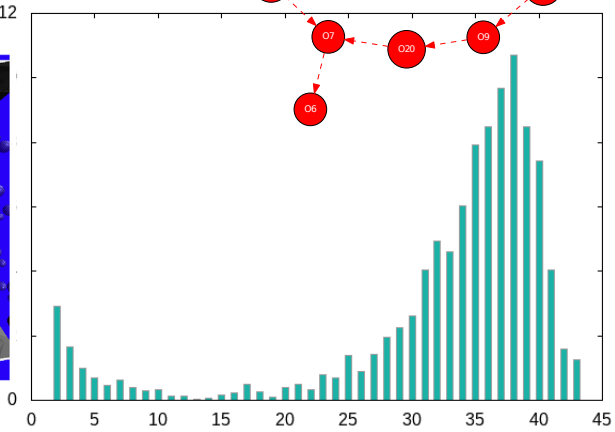
Isomorphism, connected components, Horton algo for minimum cycles
Global statistical view + time dependence of the largest component
Measure Polygon—size, connected components,

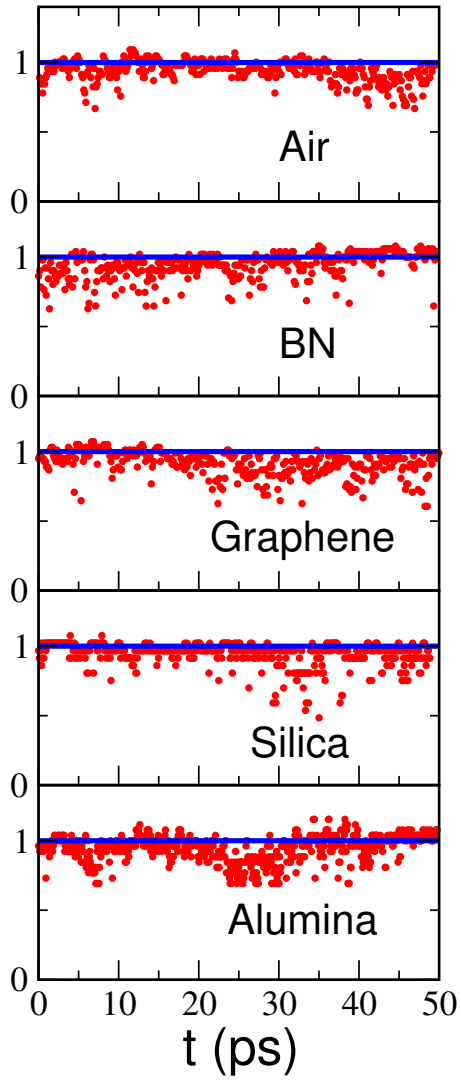








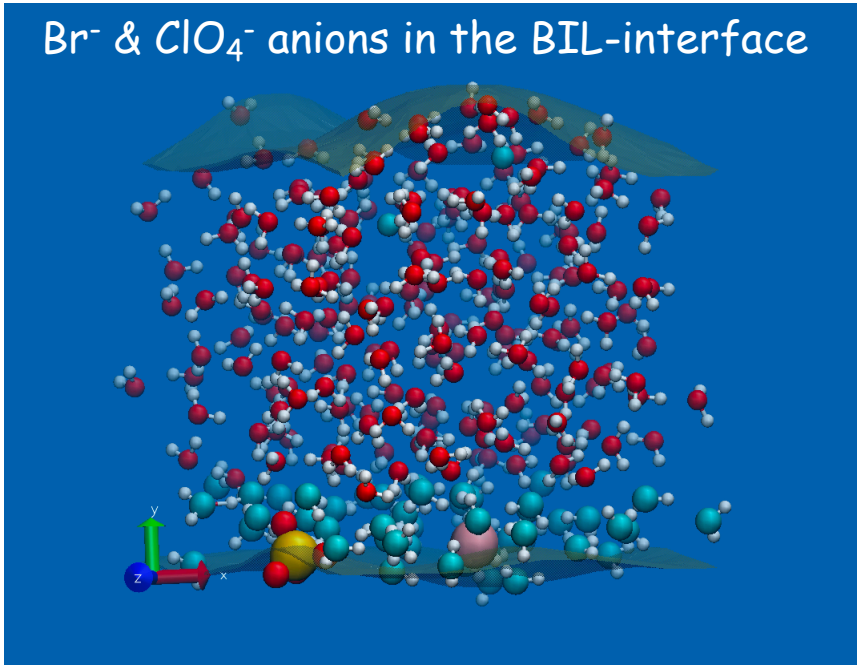


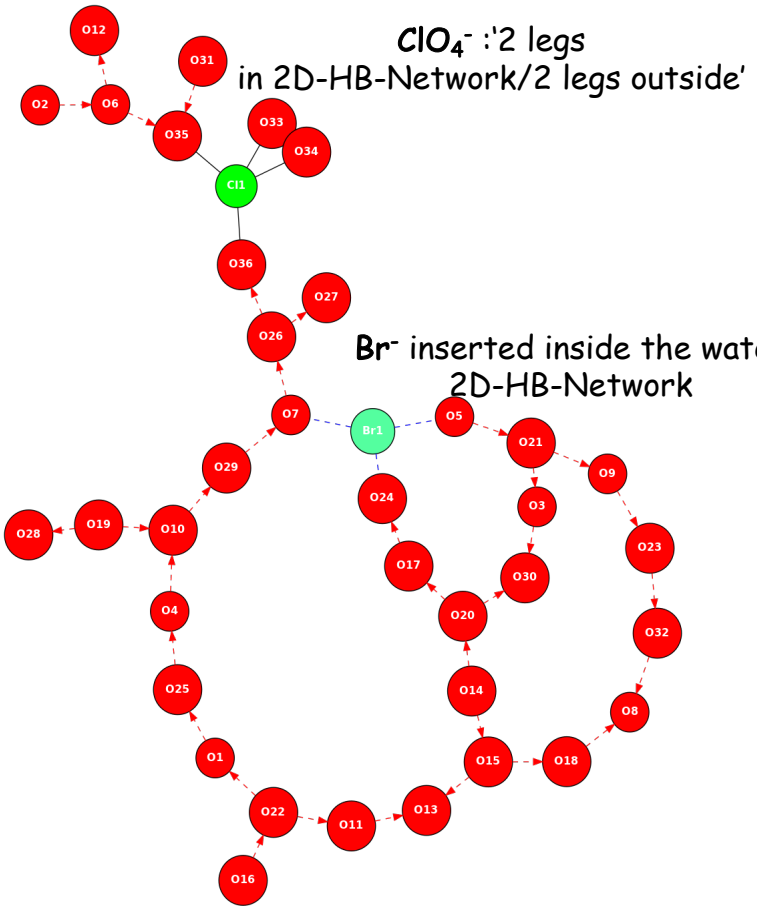


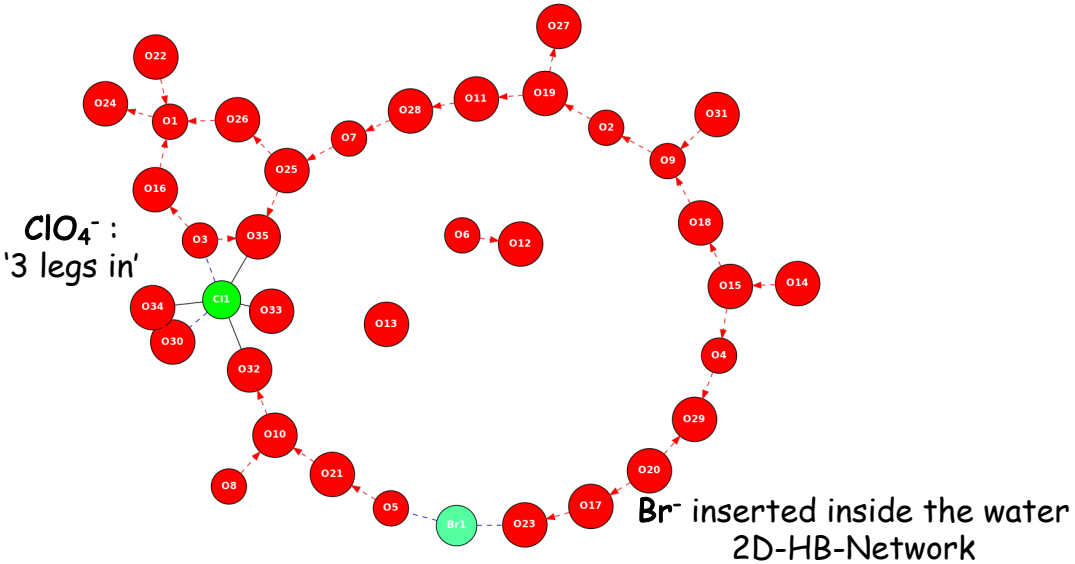
Pezzotti, Galimberti, Gaigeot, J. Phys. Chem. Letters 2017 ; Pezzotti, Serva, Gaigeot, J. Chem. Phys. 2018
Serva, Pezzotti, Bougueroua, Galimberti, Gaigeot, J. Mol. Struct. 2018 ; Pezzotti, Havenith, Gaigeot, *et al.,* J. Phys. Chem. Letters 2021

Electrolytes at the air/water interface : location ? Solvation patterns ?

Chen, Pezzotti, Bougueroua, Barth, Gaigeot
Coll. Colussi USA (Experiments)





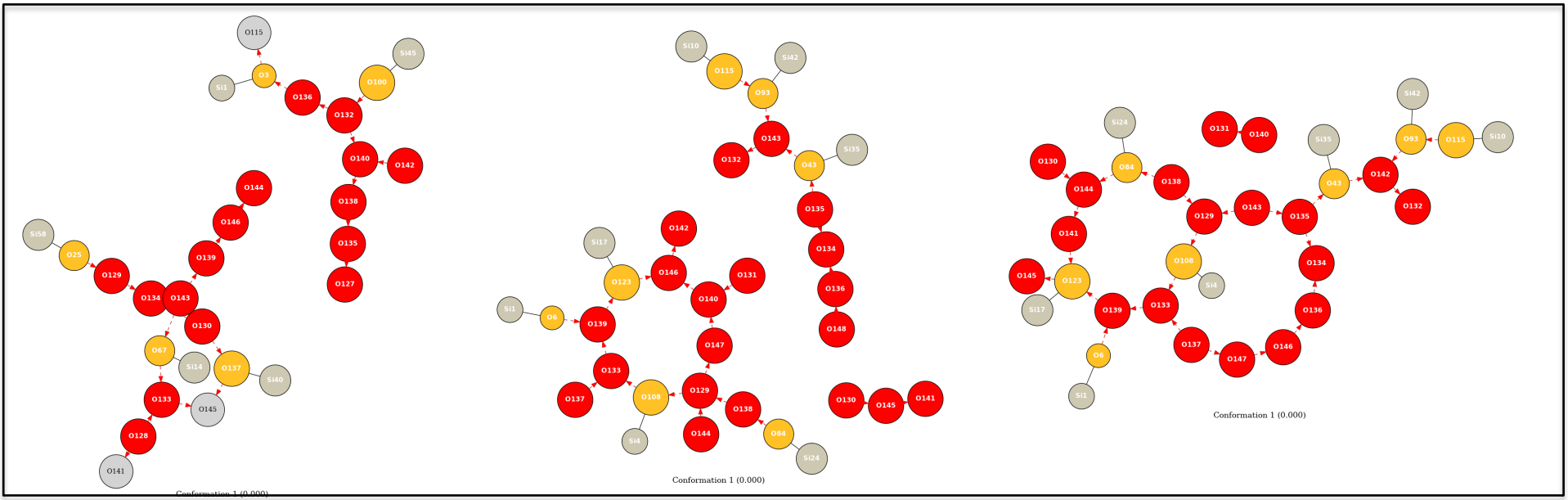


Topology of the 2D-Hbond-Network is highly dynamical

Measures of graph similarity

Solid-water interfaces and motifs at the interface

Amorphous/crystalline SiO_2 at interface with liquid water : **automatic identification of (repeated) motifs from (DFT-)MD**
From several motifs to one single motif directly measured by the 2D-MolGraphs

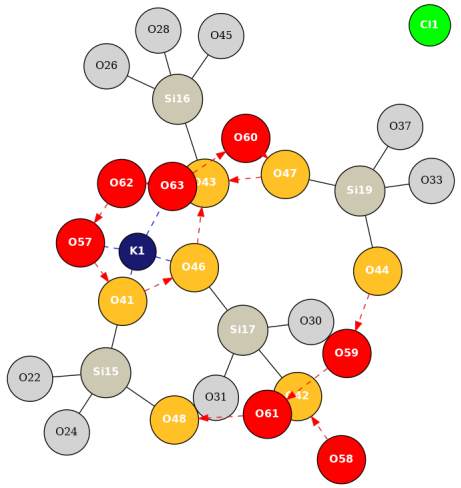


Orange & Grey balls: O & Si oxide top-surface
Red balls : Ow

Connected components
are essential

Development of algorithms
for automatic identification
of the motifs in the components of the graphs

Motifs for solvation of ions
@ Crystalline aqueous SiO2



Group 'Theory and Modeling', LAMBE UMR8587
Experts in DFT-MD, FFMD, CGMD
Experts in theoretical vibrational spectroscopies
Developers of algorithmic graph theory methods

7 permanent staff (2 PR, 4 MdC, 1 IGR)
5 PhDs, 5 Master students

Marie-Pierre Gaigeot (Group PI, Theoretical chemistry)

POSTER

Sana Bougueroua (Research Engineer, expert in graphs)

Alvaro Cimas (Assistant Prof, Theoretical chemistry)

Wanlin Chen (PhD, 2019-, Theoretical chemistry)

Quentin Bergé (M1 intern, 2022, Theoretical chemistry)

Computer sciences, Algorithmic of graphs, Laboratoire DAVID

Dominique Barth, UVSQ

Ylène Aboulfath (PhD, 2020-)

Chloé Hélain (M1 intern 2022, Computer sciences)

Coralie Zens (M1 intern 2022, Computer sciences)