M³

LAAS CNRS

In silico experiments for hybrid materials

Team Multi-level Modeling of Materials

Technology & Instrumentation for the Monitoring of Complex Systems

OBJECTIVES

> maintaining biomolecular properties in non-biological environment
> tailoring hybrid molecules with custom functions
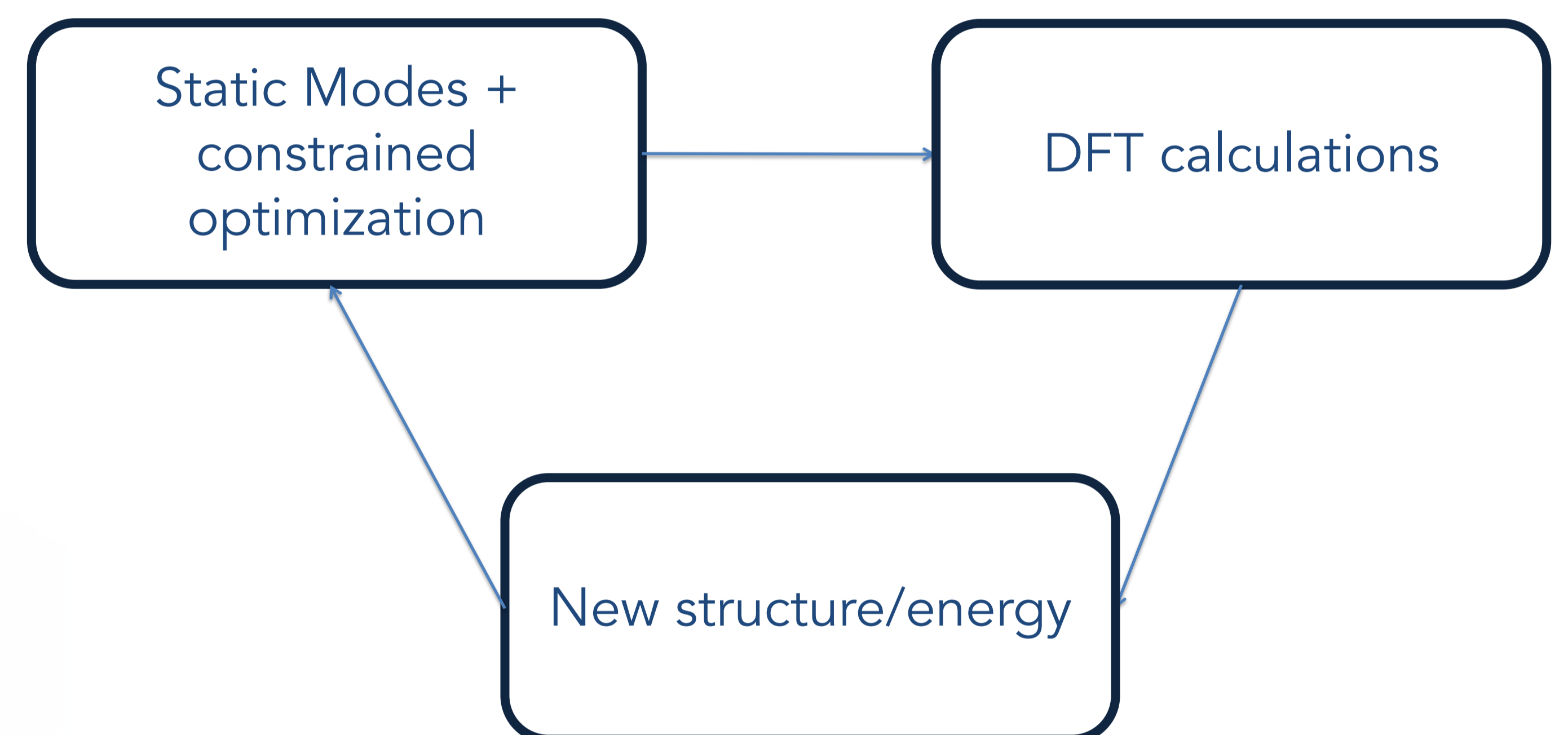> guiding innovative biotechnologies

CHALLENGES

> new methodologies for multi-scale, multi-materials systems
> biology/technology convergence
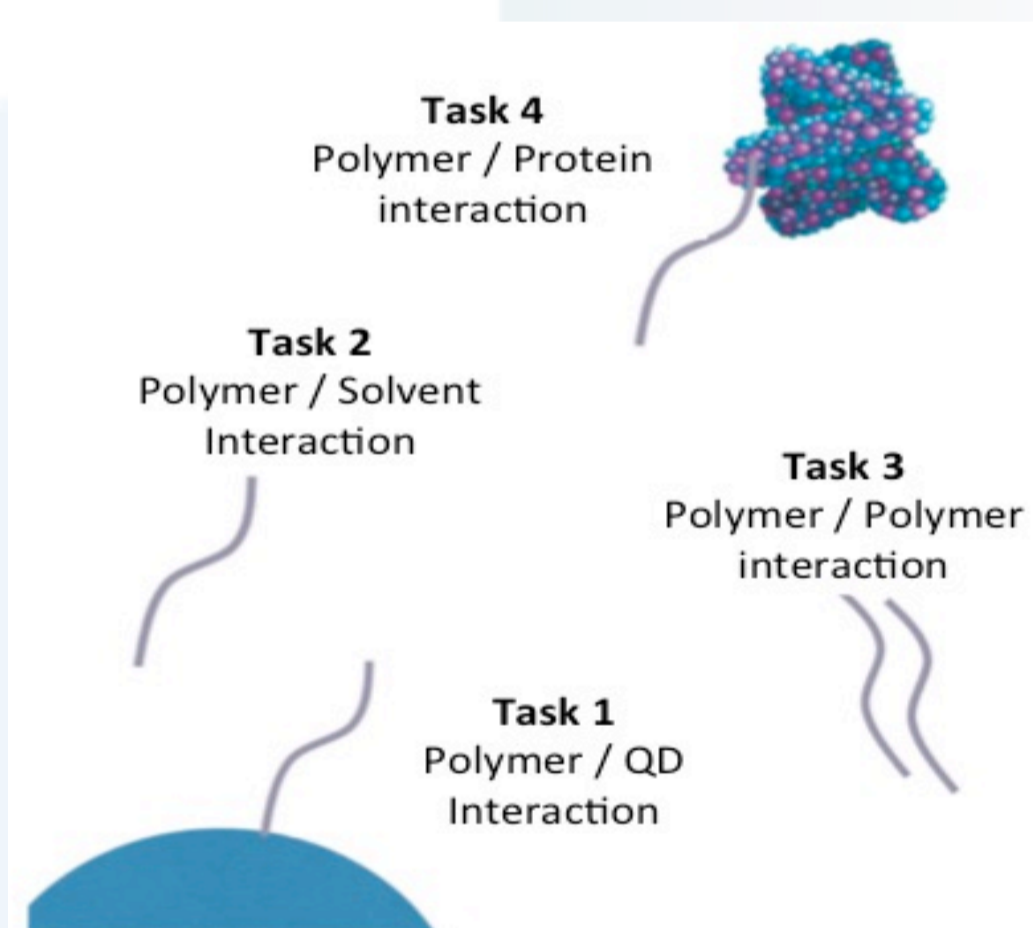
EXPERTISE & METHODS

Coupled methodologies:

- DFT based calculations
  > to predict atomic mechanisms and energy barriers

- Static Mode calculations
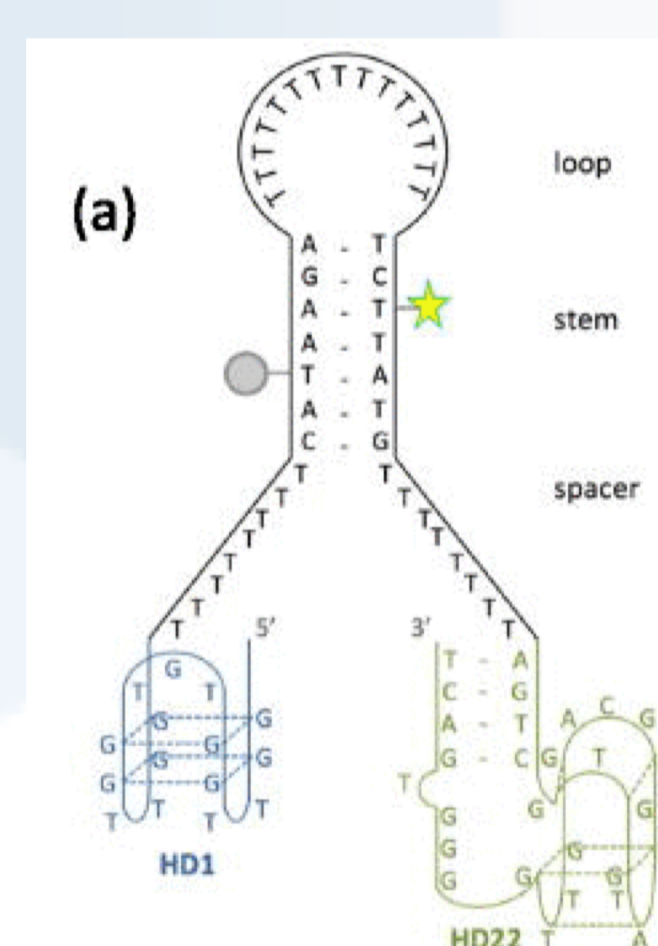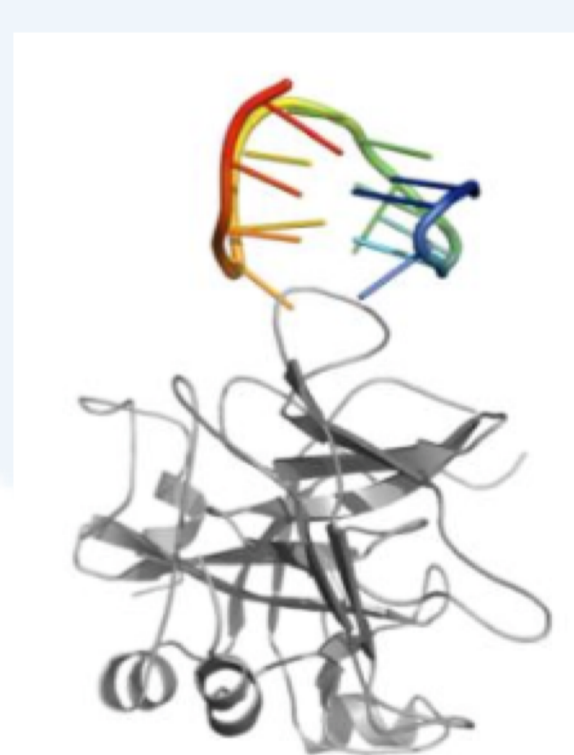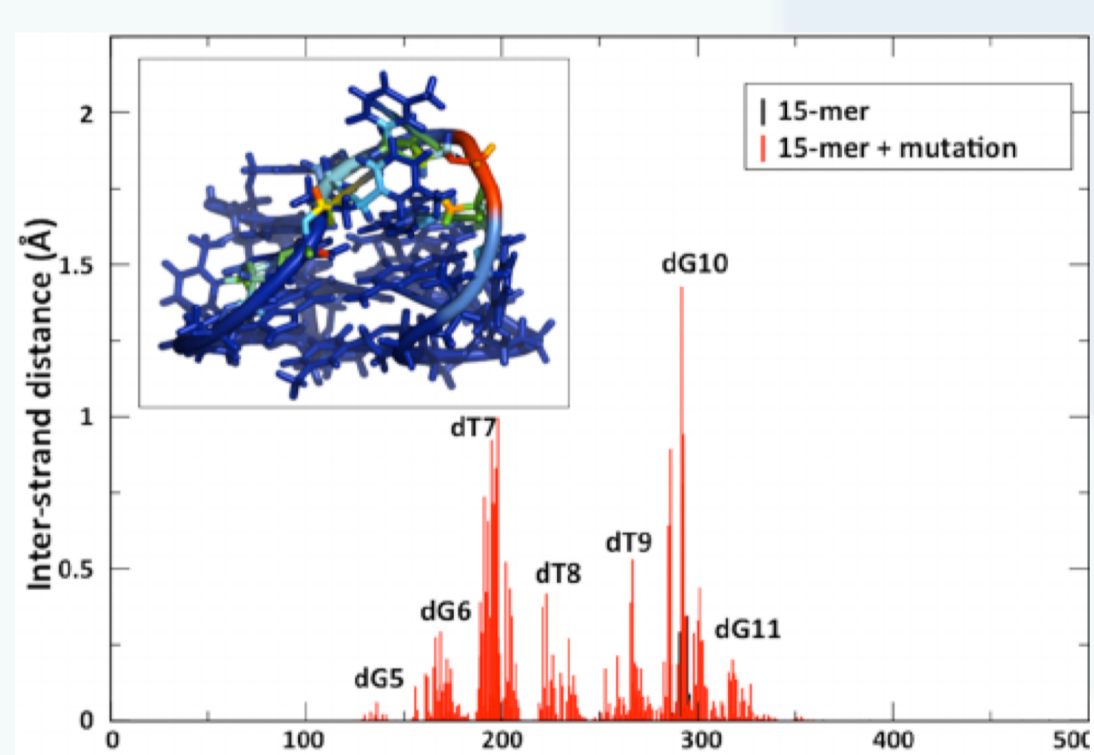 > to predict favorable pathways and skew the exploration of energy lanscape

Static Modes + constrained optimization → DFT calculations → New structure/energy →

Applications
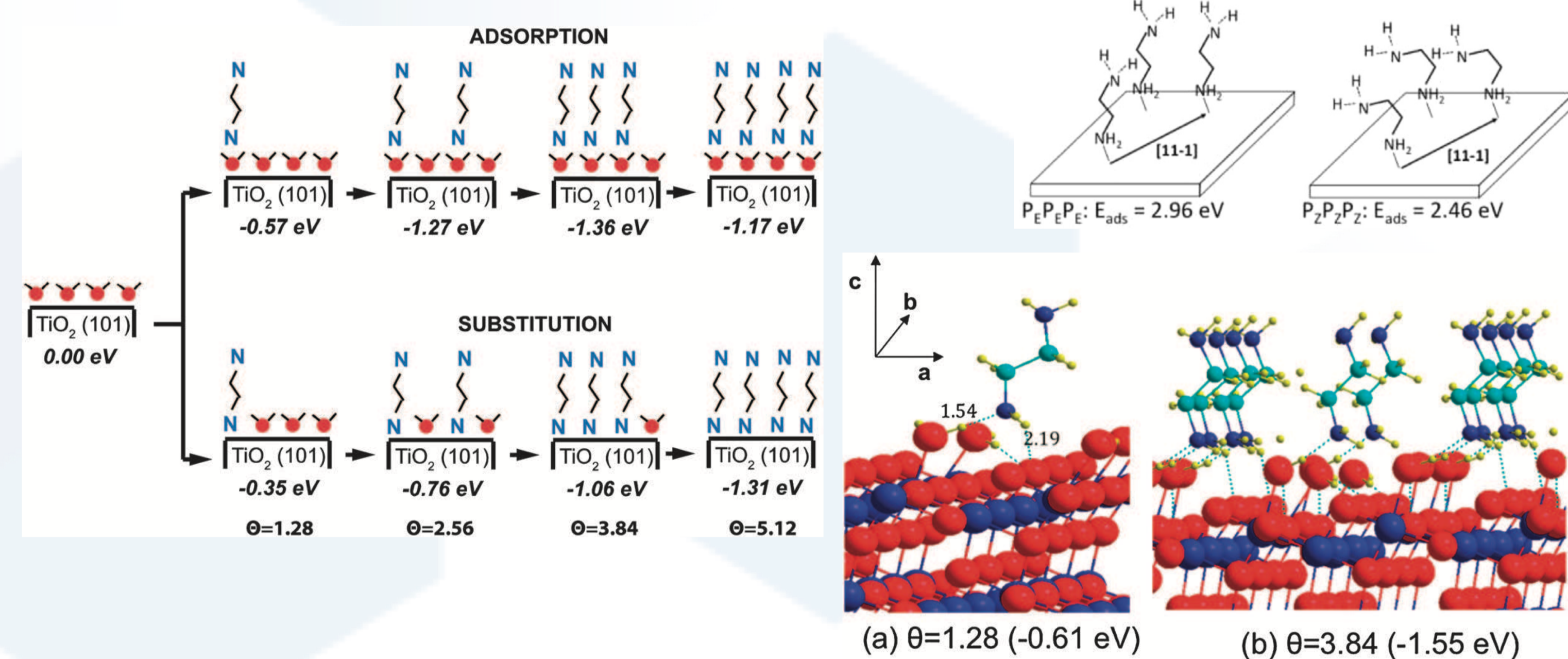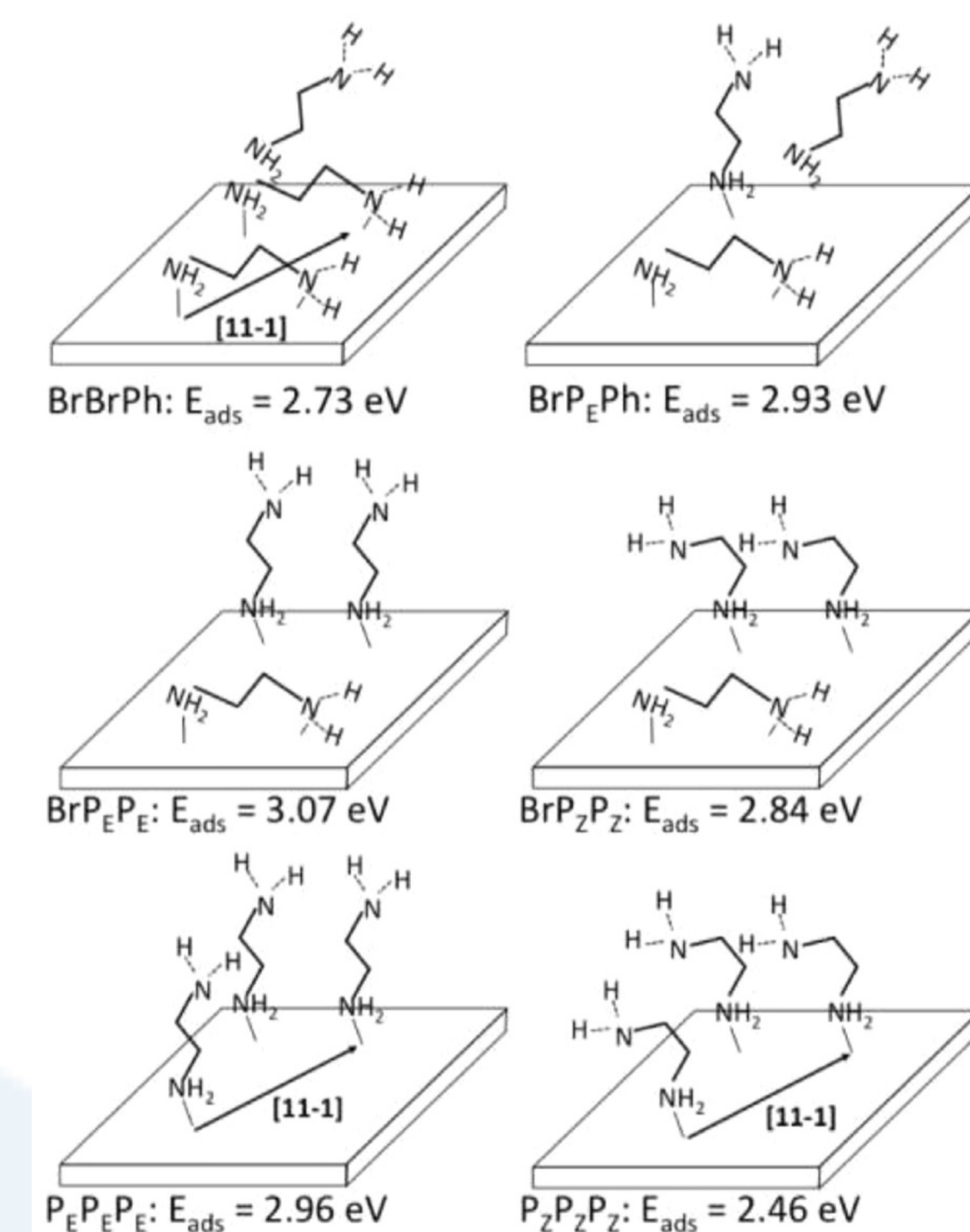
Sensing

- funtionnalized nanoparticles for bio-imaging

Task 4 Polymer / Protein interaction
Task 2 Polymer / Solvent Interaction
Task 3 Polymer / Polymer interaction
Task 1 Polymer / QD Interaction

- DNA probes for diagnosis

Inter-strand distance (Å)
15-mer
15-mer + mutation
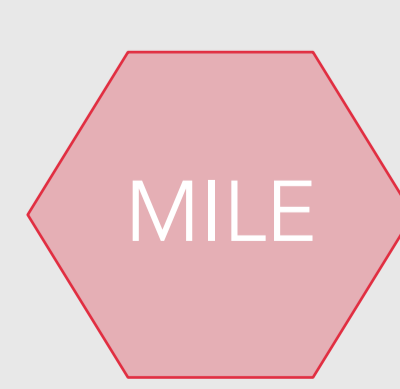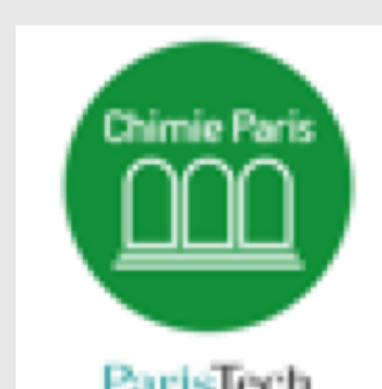dG10
dT7
dT9
dG6 dT8 dG11
dG5
Atoms

(a) loop stem spacer
HD1 HD22

Advanced versatile materials
- green coating
- organic molecules on surfaces
- (self) assembly
- corrosion inhibitors, glue...

BrBrPh: E_{ads} = 2.73 eV
BrP$_E$Ph: E_{ads} = 2.93 eV
BrP$_E$P$_E$: E_{ads} = 3.07 eV
BrP$_2$P$_2$: E_{ads} = 2.84 eV
P$_E$P$_E$P$_E$: E_{ads} = 2.96 eV
P$_2$P$_2$P$_2$: E_{ads} = 2.46 eV
[11-1]

ADSORPTION
N N N N N N N N N N
TiO_2 (101) → TiO_2 (101) → TiO_2 (101) → TiO_2 (101)
-0.57 eV   -1.27 eV   -1.36 eV   -1.17 eV
TiO_2 (101)
0.00 eV

SUBSTITUTION
TiO_2 (101) → TiO_2 (101) → TiO_2 (101) → TiO_2 (101)
-0.35 eV   -0.76 eV   -1.06 eV   -1.31 eV
θ=1.28   θ=2.56   θ=3.84   θ=5.12

1.54   2.19
(a) θ=1.28 (-0.61 eV)   (b) θ=3.84 (-1.55 eV)

PARTNERS & FUNDINGS

EDSDM ECOLE DOCTORALE SCIENCES DE LA MATIERE
IRCP Institut de Recherche de Chimie Paris
MEMS TEAM
calmip
Chimie Paris ParisTech
CIRIMAT Toulouse
MILE

REFERENCES

A. Hémeryck et al. APS 426:107 (2017)
A. Trapaidze et al. APL 107:233701, (2015)
A. Hémeryck et al. PCCP 15:10824 (2013)
M. Brut et al. APL 100:163702 (2012)

anne.hemeryck@laas.fr
marie.brut@laas.fr