

Knowledge on:

1. Thermodynamics and Statistical Mechanics

2. Statistics and Data Analysis

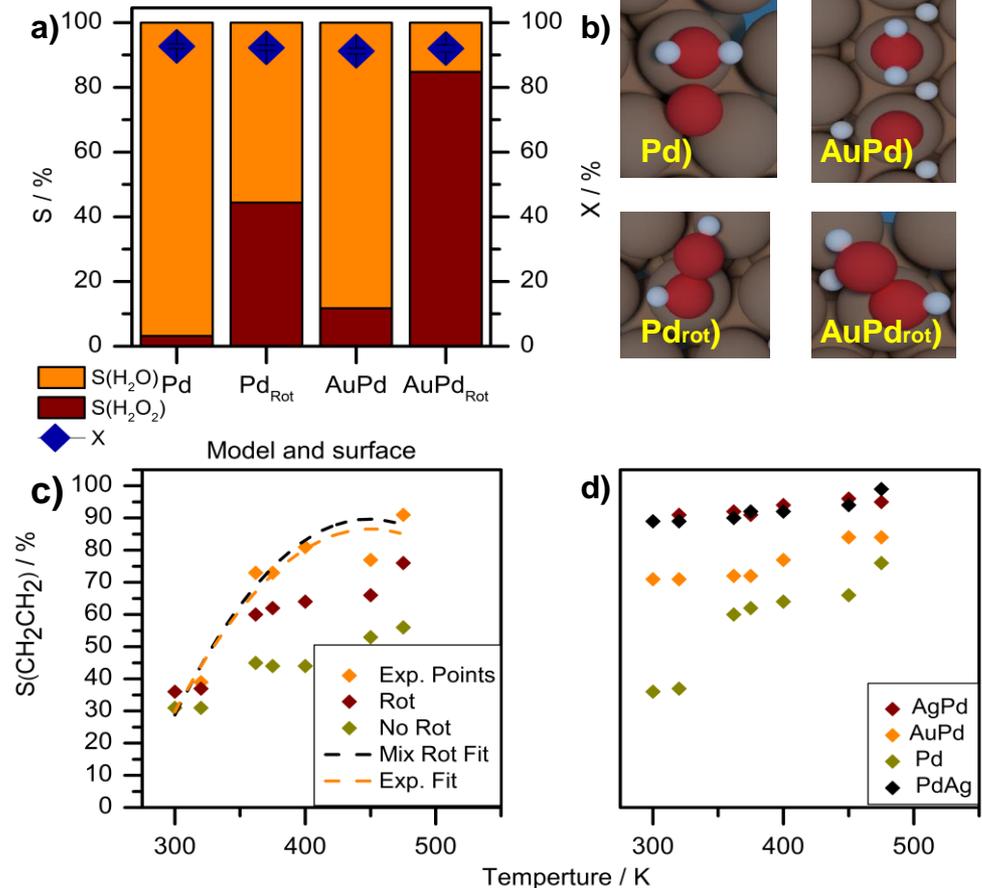
Main programming language:
C++

Some knowledge on:

1. LaTeX and Beamer

2. Python language (for beginners)

3. Blender (for beginners)



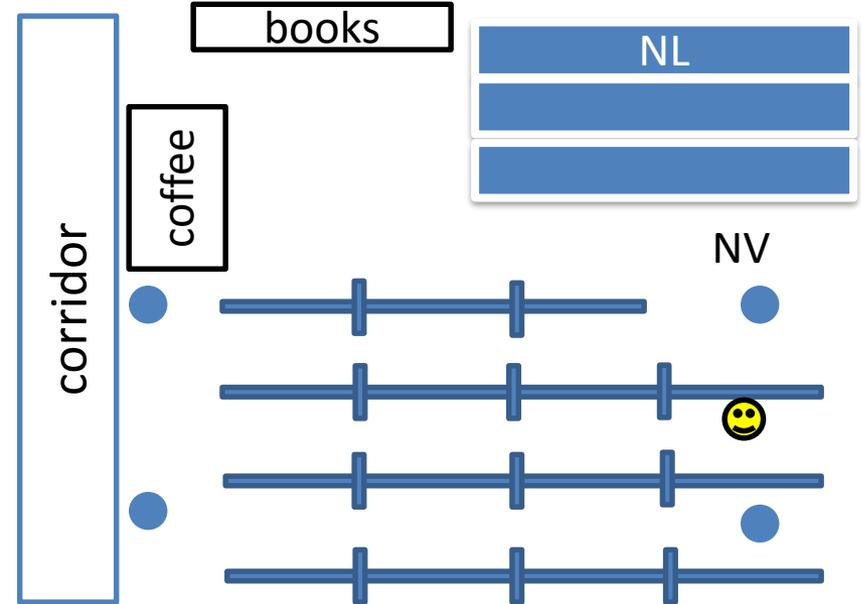
Bob



Physicist

Expertise

- Statistical physics, Data analysis
- Quantum transport modelling
- Oxygen evolution reaction
- Quantum Espresso, CPMD
- Python, Fortran, Mathematica
- GIMP, Material Studio
- SIESTA, LAMMPS, CP2K, Matlab, Bash
- Gold Nanoparticle functionalization
- Non-Equilibrium Green Function
- Bioinformatics, Machine Learning
- Risk management
- Translational medicine



Will gladly offer help with

- Those
 - Driving you to the spa (as long as we are an even number)
 - Emergency chocolates

Will reluctantly help you with

- These
 - French, German, English
 - Paperwork
 - Emergency first aid

Single Atoms on Carbon Supports

Edvin Fako

WAS CALCULATING:

- contain: C, N, Au or Pd
- VASP; PBE; D3
- "converge nicely"
- unique behaviors

CAN HELP WITH:

- interpreting EXP
- analyzing MD
- simulating XPS
- radial dist. + EXAFS

SCRIPTING:

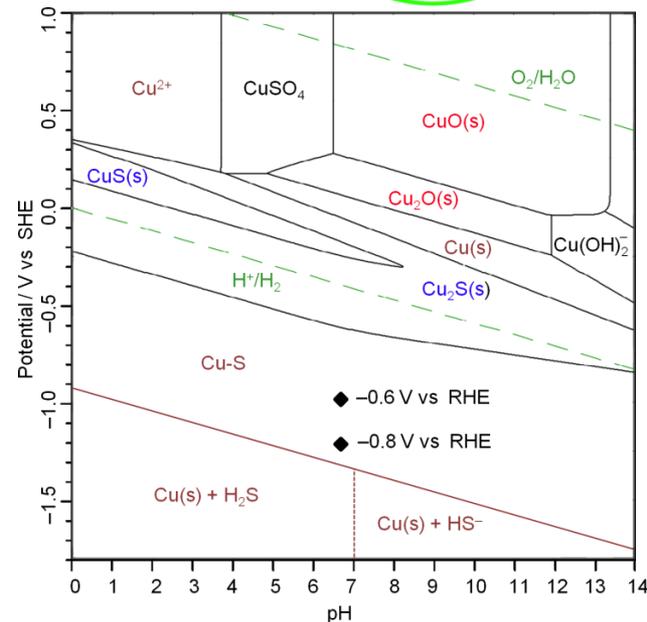
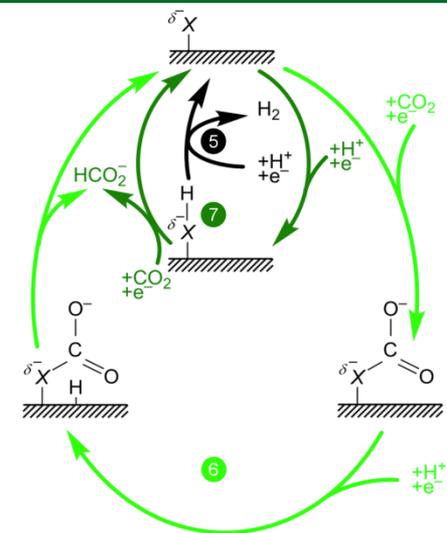
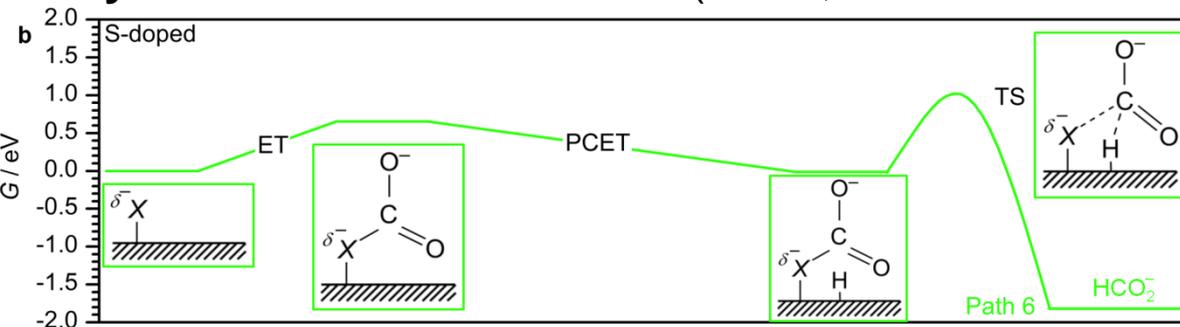
- BASH
- Python
- Tensor Flow
- miscellaneous

DEFINITELY CHECK OUT:

- PANDAS (python module)
- Blender (3d rendering tool)
- Inkscape (vector graphic editor)

DFT in electrochemical systems:

- Electric potential (*Computational Hydrogen Electrode*);
- Energy profiles (*OriginPro*); $\Delta G_n(U) = \Delta G_n(U = 0) + neU$
- Reaction schemes (*ChemDraw*);
- Pourbaix Diagrams (*HydraMedusa*);
- Crystal structures/surfaces (*ICSD, Materials Studio*).



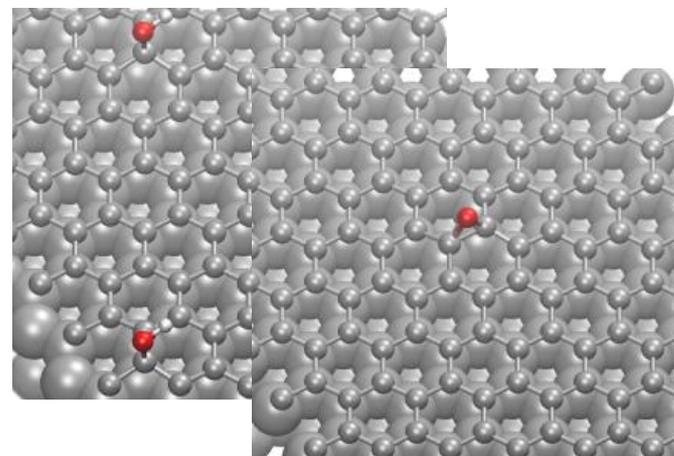
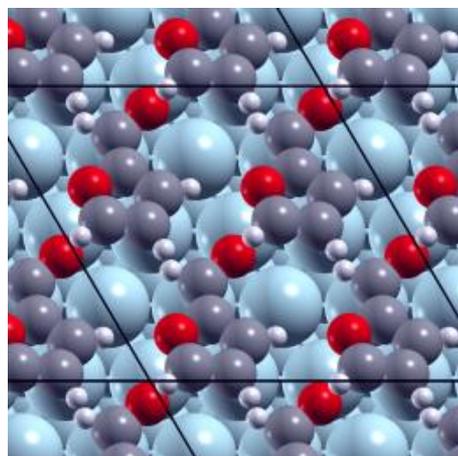
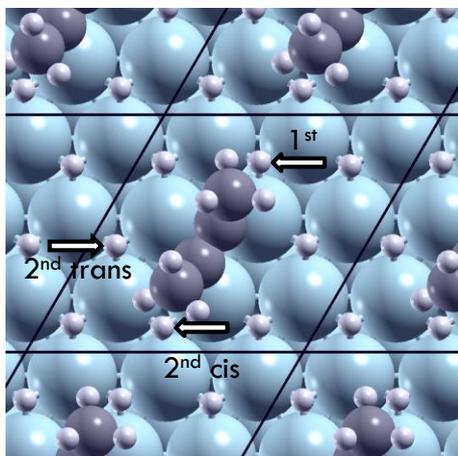
Additional skills:

- Availability for external issues;
- Travel organization;
- *Science Outreach*.



■ Expertise

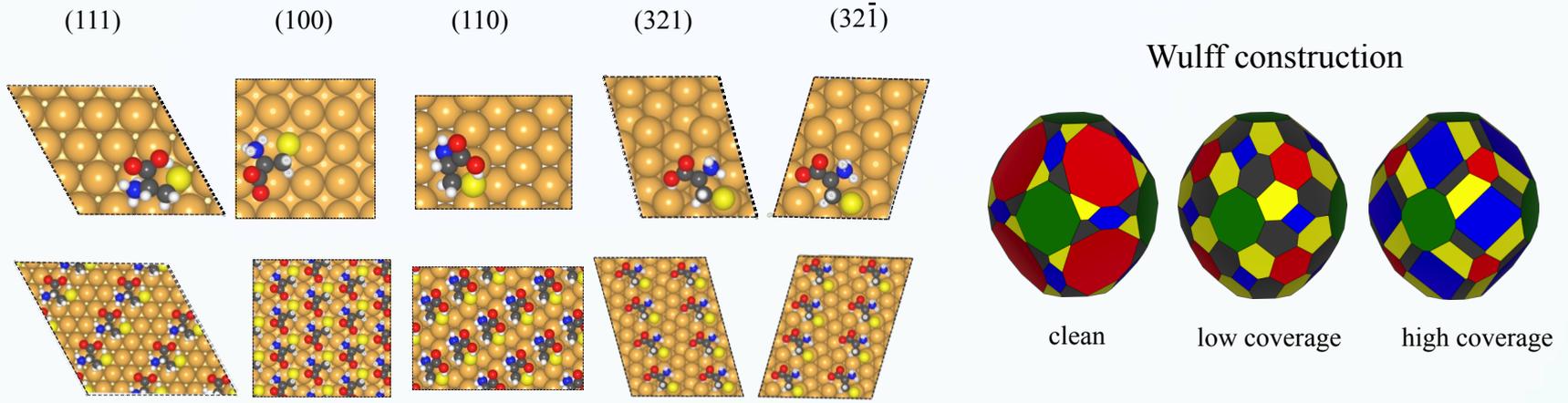
- Reaction mechanisms on densely packed environments
- Physicochemical properties: structural (cell), vibrational (IR, RAMAN), electric (charges), spectroscopic (XPS)



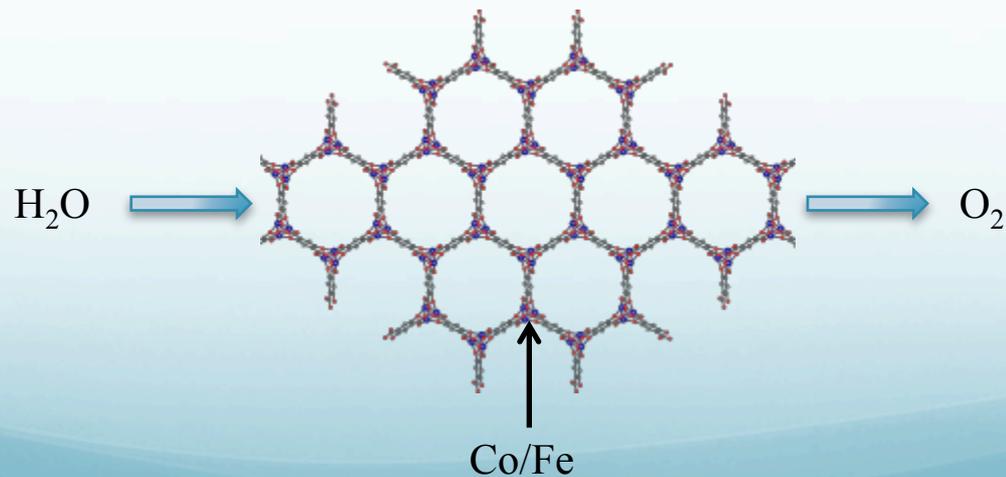
■ How can I help

- Design of potential reaction pathways at high coverage
- Surface characterization and functionalization

First-Principles Study of Chiral Shape Induction in Gold Nanoparticles by L-Cysteine Amino Acids



Modeling of Metal-Organic Frameworks for OER





- Finding the structures (.cif)
- Extracting and processing of data
- “In situ” comparison of calculated and experimental data

System	Elem	no.	Sym	en-1	en-2									
fe1p1:	Fe P	4 4	Pnma	-59.30416811	-59.40362645	5.1548	3.0488	5.7588	5.191	3.099	5.792	8137	'P n m a'	
fe1p2:	Fe P	2 4	Pnmm	-41.33049674	-41.33049350	4.9600	5.6428	2.7198	4.9729(7)	5.6568(8)	2.7230(4)	8815	'P n n m'	
fe1p4:	Fe P	8 32	C12/c1	-253.83519446	-253.83520497	5.0581	10.4152	11.1004		5.0543(7)	10.407(2)	11.069(2)	844	'C 1 2/c 1'
fe2p1:	Fe P	6 3	P-62m	-69.16777972	-69.81072349	5.8046	5.8046	3.4290	5.69(6)	5.69(6)	3.458(2)	7712	'P -6 2 m'	
fe3p1:	Fe P	24 8	I-4'	-248.34611251	-250.02401366	8.8879	8.8879	4.4201	9.107(2)	9.107	4.460(1)	449	'I -4'	
fe4p1:	Fe P	4 1	Pmmm	-33.97003563	-36.28559705	4.1467	4.1444	4.1438	3.59(5)	4.01(5)	4.32(5)	11119	'P m m m'	
fe-bu:	Fe	2	Im-3m	-15.52844433	-16.47762430	2.8317	2.8317	2.8317	2.8665(2)	2.8665	2.8665	141414	'I m -3 m'	

- Identifying of different species of the same element in crystals
- Dencity of states, band centers
- Cleaving (Materials studio)
- Surface energy, workfunction
- Segregation, islanding
- Phosphide crystals
- Giving directions who can explain it better

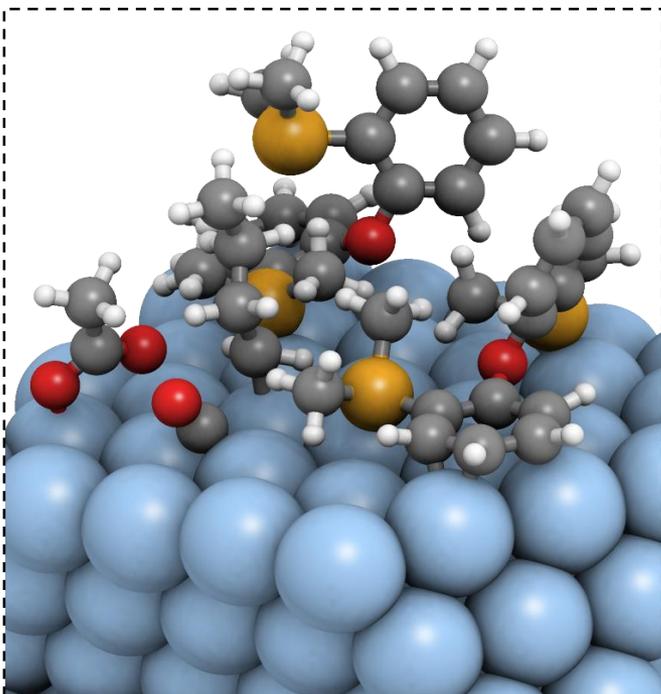


Experimental background

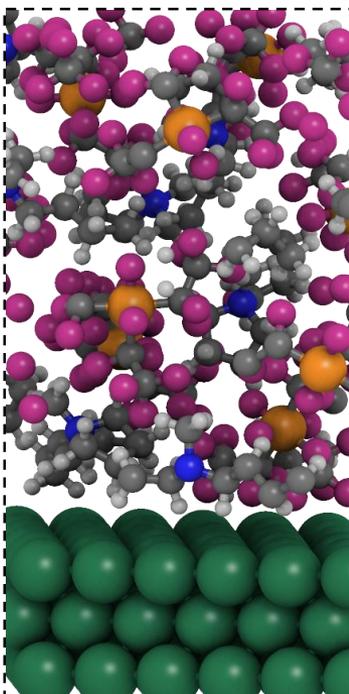
- GC-MS, ICP-OES, ICP-MS, AAS...

I also know how to make la tortilla de patatas (good one)

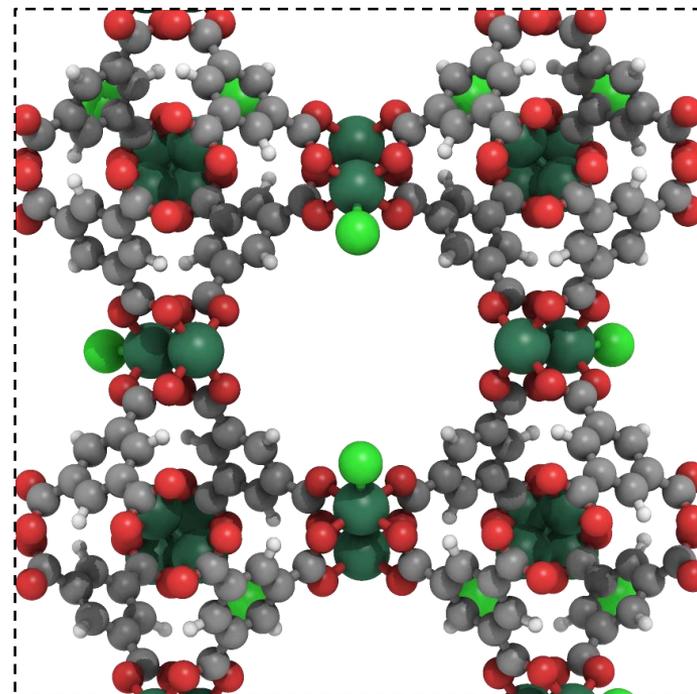
Ligand-decorated metals



Interfaces



Porous materials



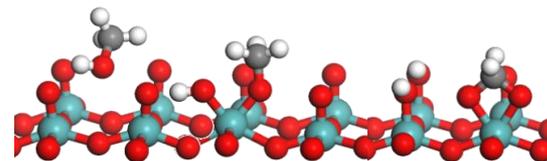
How can I *further* help?

- > System: homogeneous (organometallic) catalysis, open-shell systems
- > Software: Gaussian (DFT), CP2K (ab initio MD), LAMMPS (classical MD)
- > Support: dissemination/outreach, writing of proposals, etc.

Marcos Rellán

Who I am?

- **Background:** PhD thesis about reactivity on RTMO's (MoO_3)
- **Current work:** industrial collaboration (Covestro)



What can I offer you?

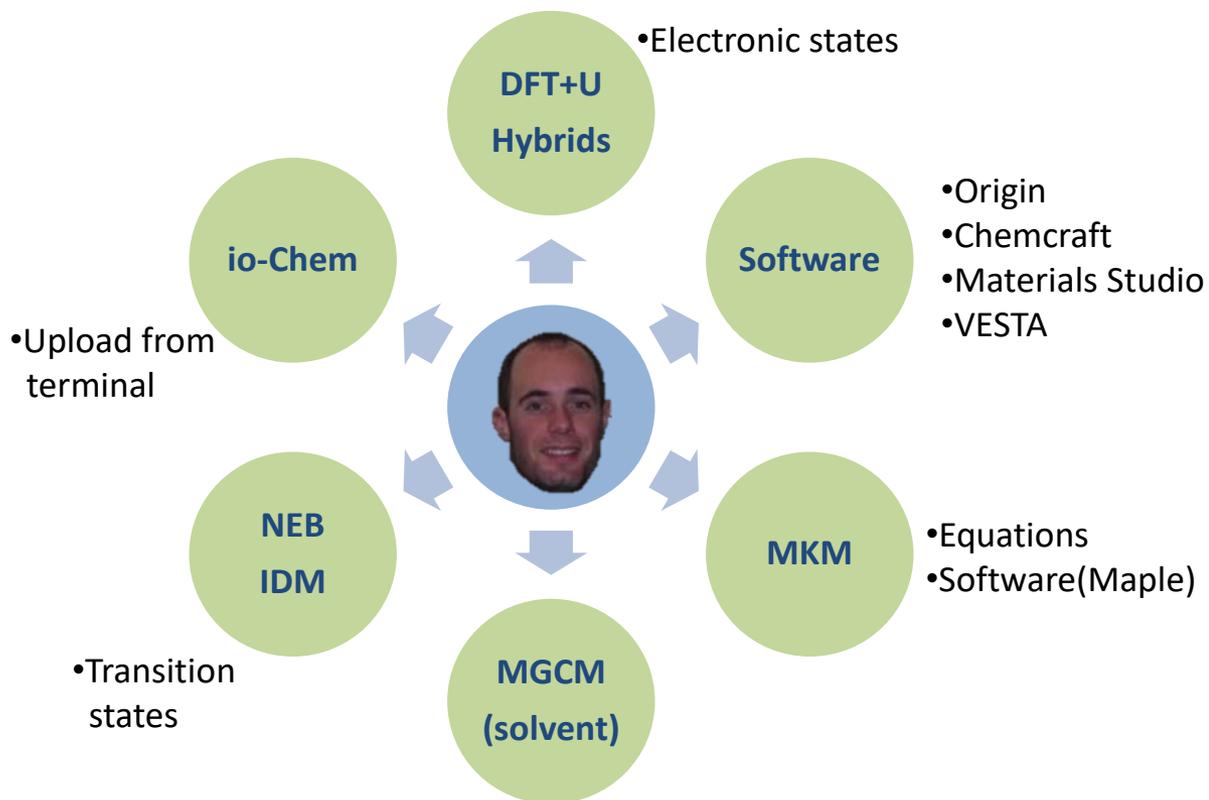
KNOWLEDGE &
EXPERIENCE

5 years in this group!!



I can book meeting rooms

You can ask me about...



Nathan Daelman (Msc. Theoretical Chemistry)

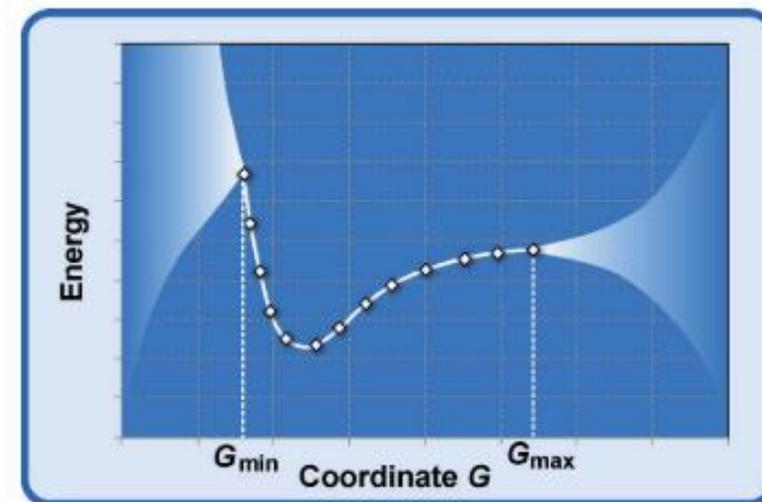
CO₂ IN
VASP

• Computational Chemistry:

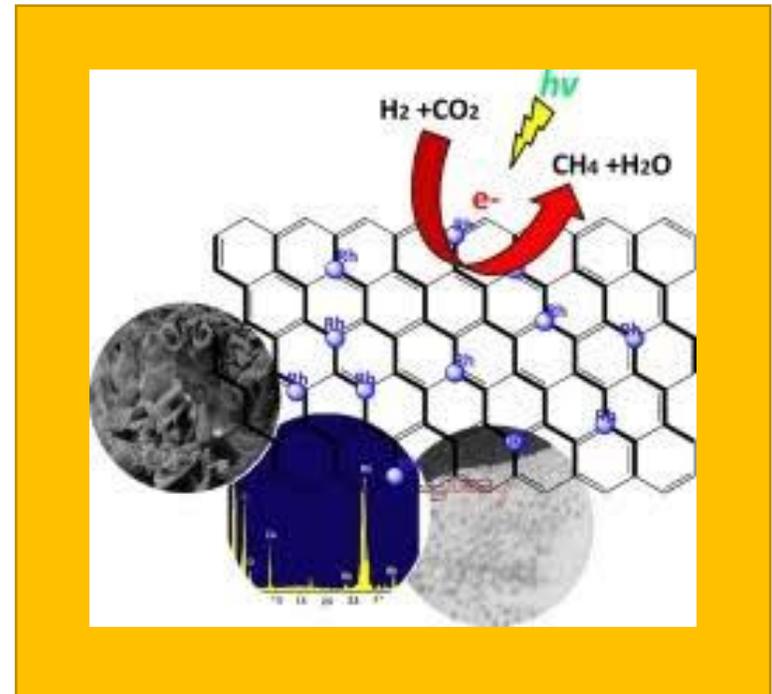
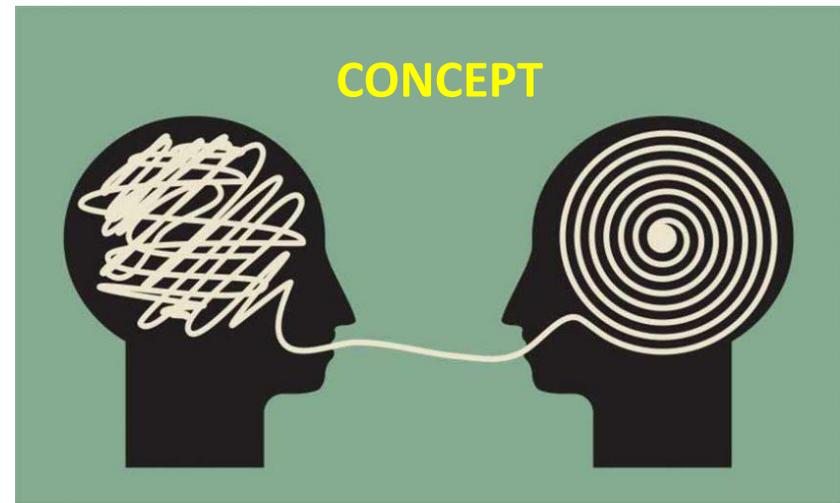
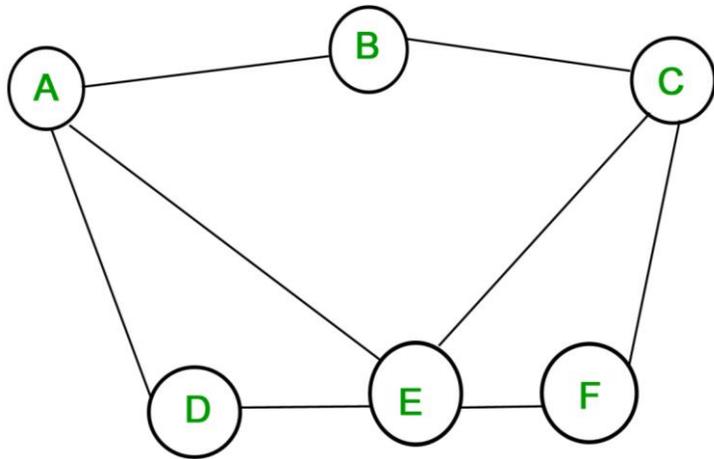
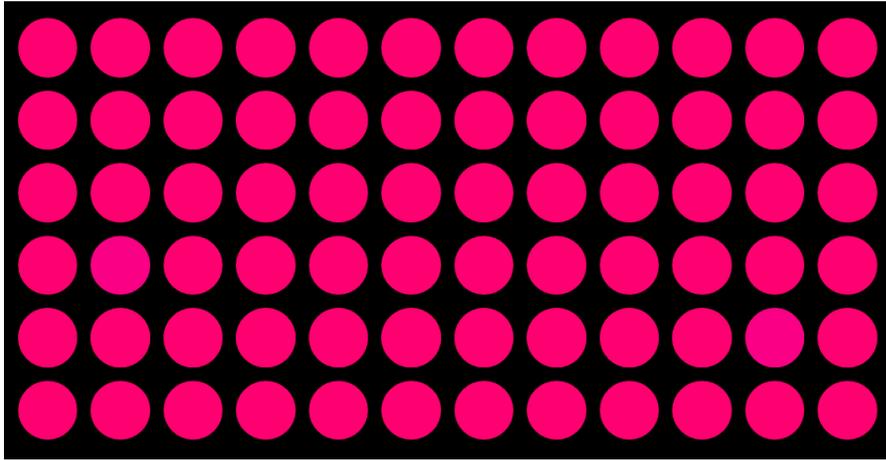
- BOMD
- Dimer
- Core-level Binding (XPS)
- Bader
- GW
- RPA (ACFDT)

• Machine Learning:

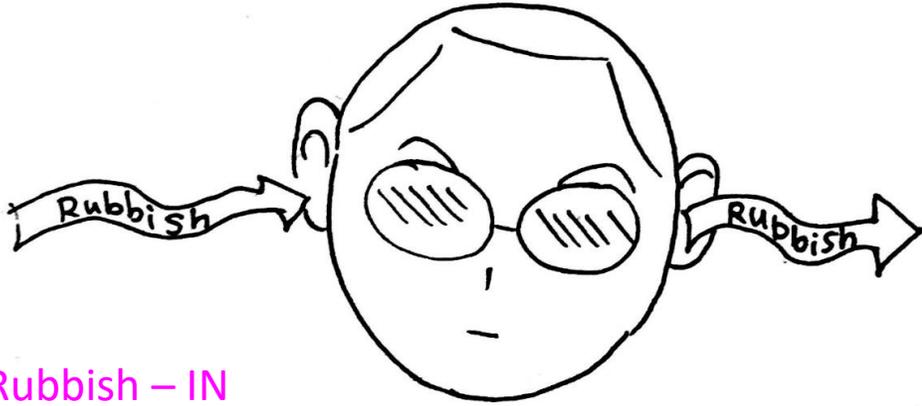
- Stanford On-line Course (completed)
- (Behler-Parinello) Neural Network Potentials
- **Programming:** Python2.7, Fortran90/95, Bash, Perl, Awk
- **Graphic design:** Blender, Gnuplot, Photoshop/Gimp
- **English grammar/spell check**



PAULINA PRŠLJA



The Q-robot



Rubbish – IN

- INCAR: ALGO, ISMEAR, vdW, DFT+U, EDIFF(G);
- KPOINTS: HCP(Γ -centered), K^*a , Line mode;
- POSCAR: Structure with Physical meanings;
- POTCAR: Consistent with POSCAR, M_{sv} , M_{pv} ;
- Script: which queue, vasp_version, how many cores?

Rubbish – OUT

- Errors/Wrong Results/Hanging in the queue
- None-Physical geometric and electronic structures
- Waste time/resources (Not only Yours!!!)

What is Q-robot?

- A bunch of python/bash scripts with element operations;
- A **DIY** Assistant; A **TRUSTED** Friend (Not only tools);
- An intelligent **Chemist** (Perhaps in the future).

What Can Q-robot do?

- 1) Check/Generate initial inputs (Avoid Rubbish--IN);
- 2) Build geometries from commands (supervised model);
- 3) Analysis outputs (Geometric, Electronic)

Example: xps.py; d2-dict.py, e6.py, check.py, opt.py, neb.py
fix.sh, translate.py, rotate.py, copy.py, del.py, add.py;
dos_extract.py, entropy.sh, band.py, etc.

Where to find the current version of Q-Robot?

- 1) aliga.iciq.es/wiki; 2) /home/qli/bin; 3) ask me directly.

What will Q-robot do in the future?

- 1) Analyze the task and Provide the best strategy;
- 2) Automatically generate the tasks (unsupervised model);
- 3) Supervise the calculation by itself and generate the report;
- 4) Analysis outputs in a Chemist view.

Rodrigo García-Muelas

Strong skills:

- * Maths, **Linear Algebra**
- * (Micro)kinetic modelling

Experience:

- * Bash & Python 3
- * Fortran
- * Maple, Excel

In development:

- * Statistical Learning: PCA, Random Forest, etc.
- * Microkinetics in Maple (w/ Qiang Li).
- * List of colours for internal use.
- * **Core-level shifts / XPS.**

Always comment your code

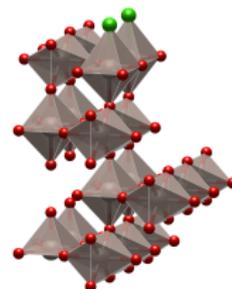
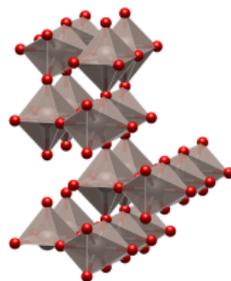
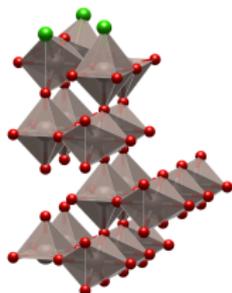
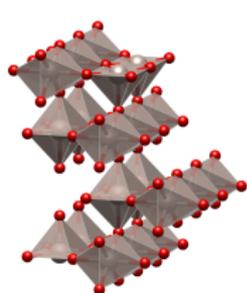
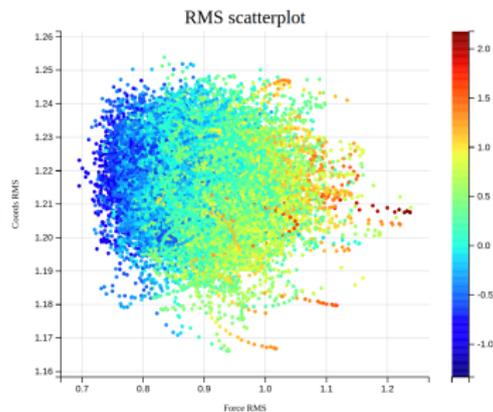
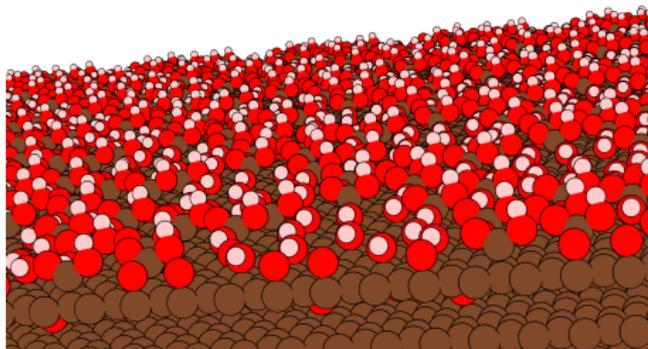
pyRDTP

- Aims to read and build geometries for/from VASP.
- Contains a set of tools in order to analyze and process catalytic system geometries.
- Can generate large sets of geometries using simple "recipes".
- Coded in Python 3.

Mephistopheles

- Daemon that aims to control complex Workflows via flexible modules.
- Complements Fireworks. Adds flexibility and dependency management.
- Used along with pyRDTP to build, compute and analyze large sets of calculations.
- Can communicate with external software and act in consequence.

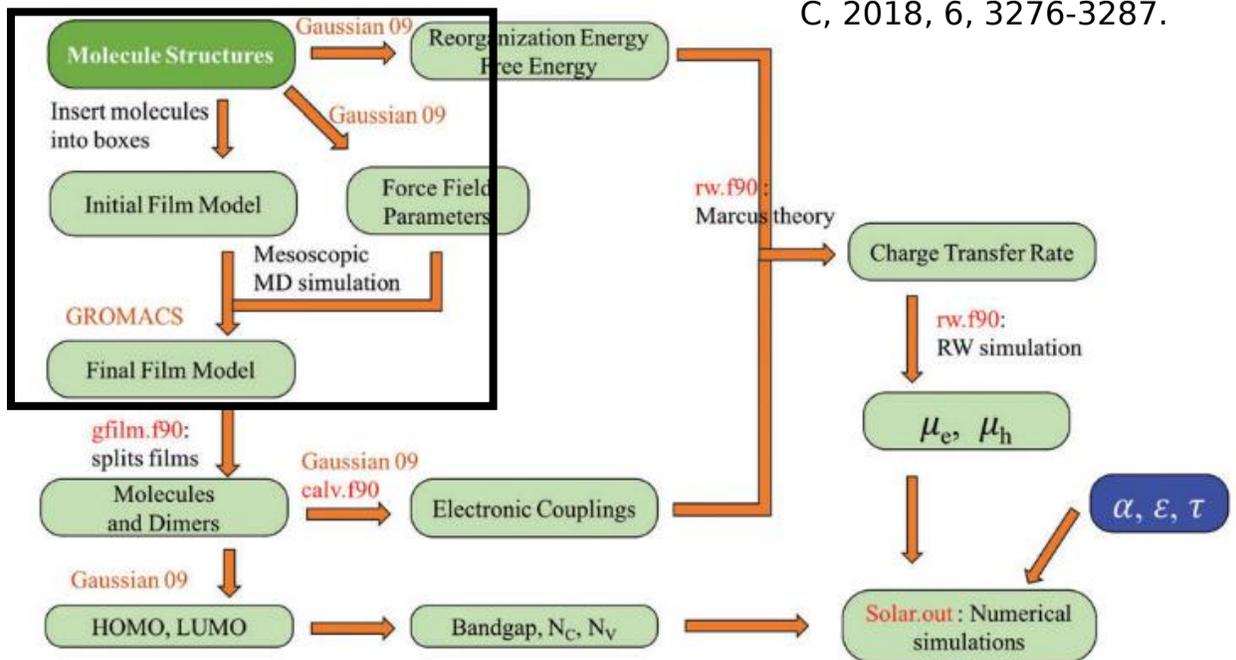
Applications



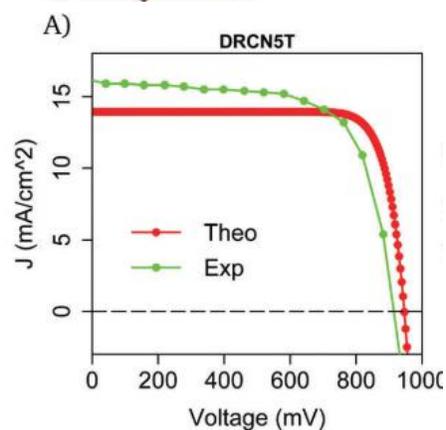
Yecheng Zhou

- Physics- Semiconductor physics
- Building Multiscale Models
- Fortran programing with MPI

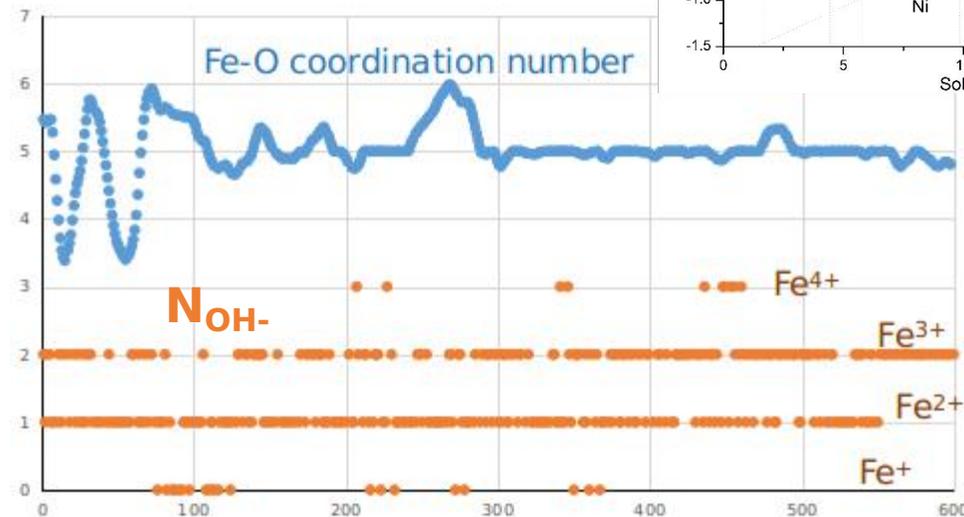
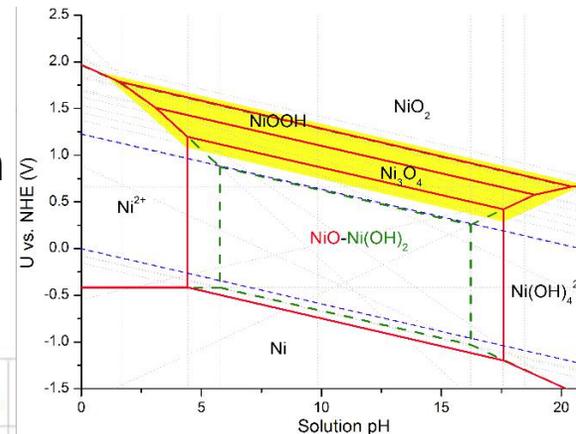
Y. Zhou et al. J. Mater. Chem. C, 2018, 6, 3276-3287.



Molecule	J_{sc}	J_{sc} EXP	V_{oc}	V_{oc} EXP	PCEs	PCEs EXP
DRCN5T:P C71BM	13.9	15.7	0.92	0.95	10.8	9.8
DRCN7T:P C71BM	12.3	14.9	0.91	0.74	7.5	9.1
DERHD7T: PC71BM	11.5	9.5	0.89	0.65	5.9	5.9



- Pourbaix diagram
- CP2K AIMD simulation
- VASP-MGCM



Larger ENCUT
and NX*NY*NZ

Versions	N-NCPU	E (eV)	ENCUT
Old	C12-48	failed	400
Old	C28	-199.41	550
Revised	C12-48	-199.54	750

Faster

Node-Cores	Relaxation(S)	STC(S)	Etotal (eV)
c8-16	23484.48	6713.72	-278.28574
c12-24	19381.68	4708.82	-278.28574
c28-28	3496.83	2908.43	-278.28574

Job script: /home/yzhou/bin/rvaspmsgcmc28