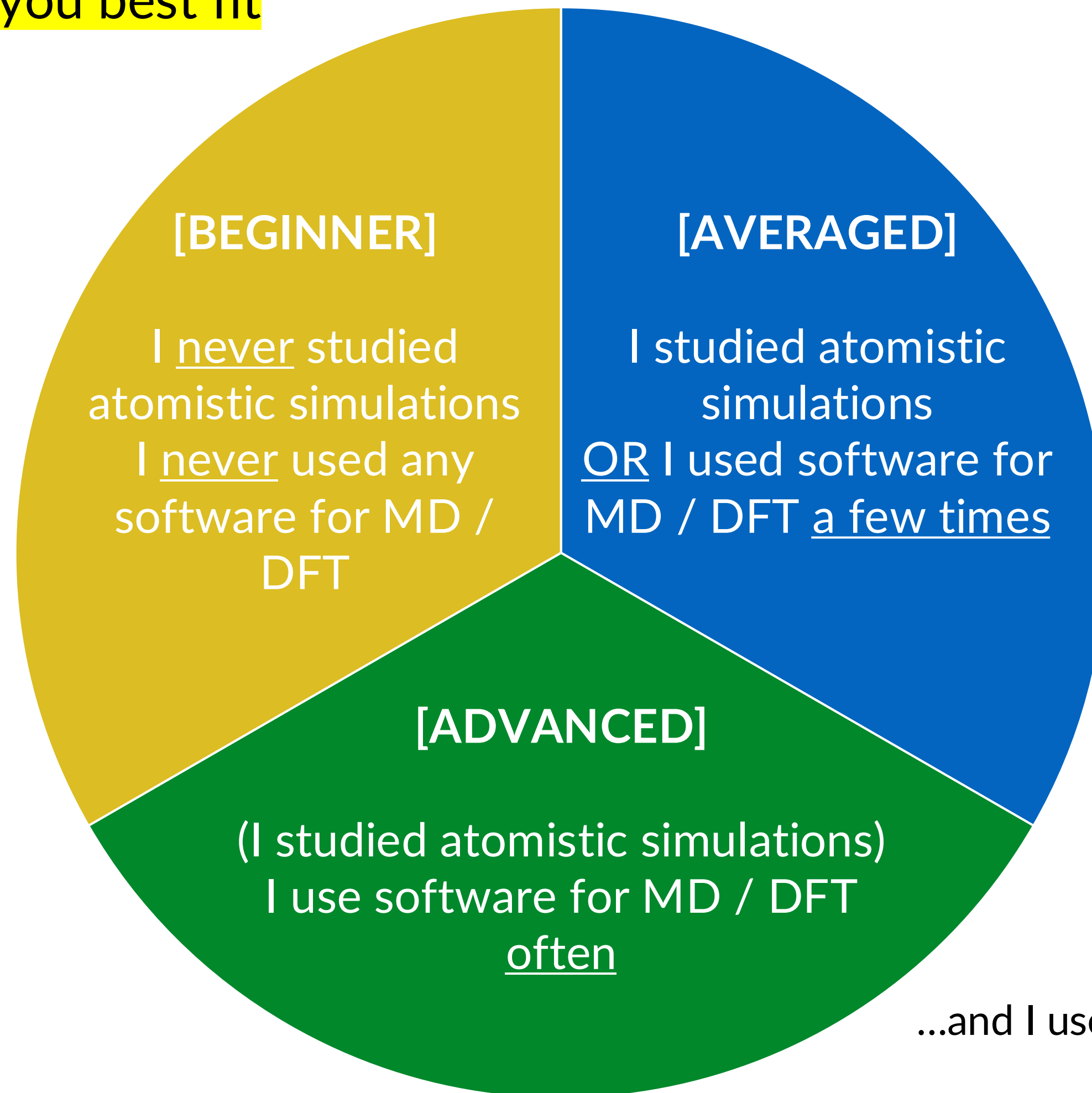


AMS Workshop: Using the Amsterdam Modeling Suite on SURF Research Cloud

Nicolas Onofrio, Software for Chemistry & Materials
onofrio@scm.com

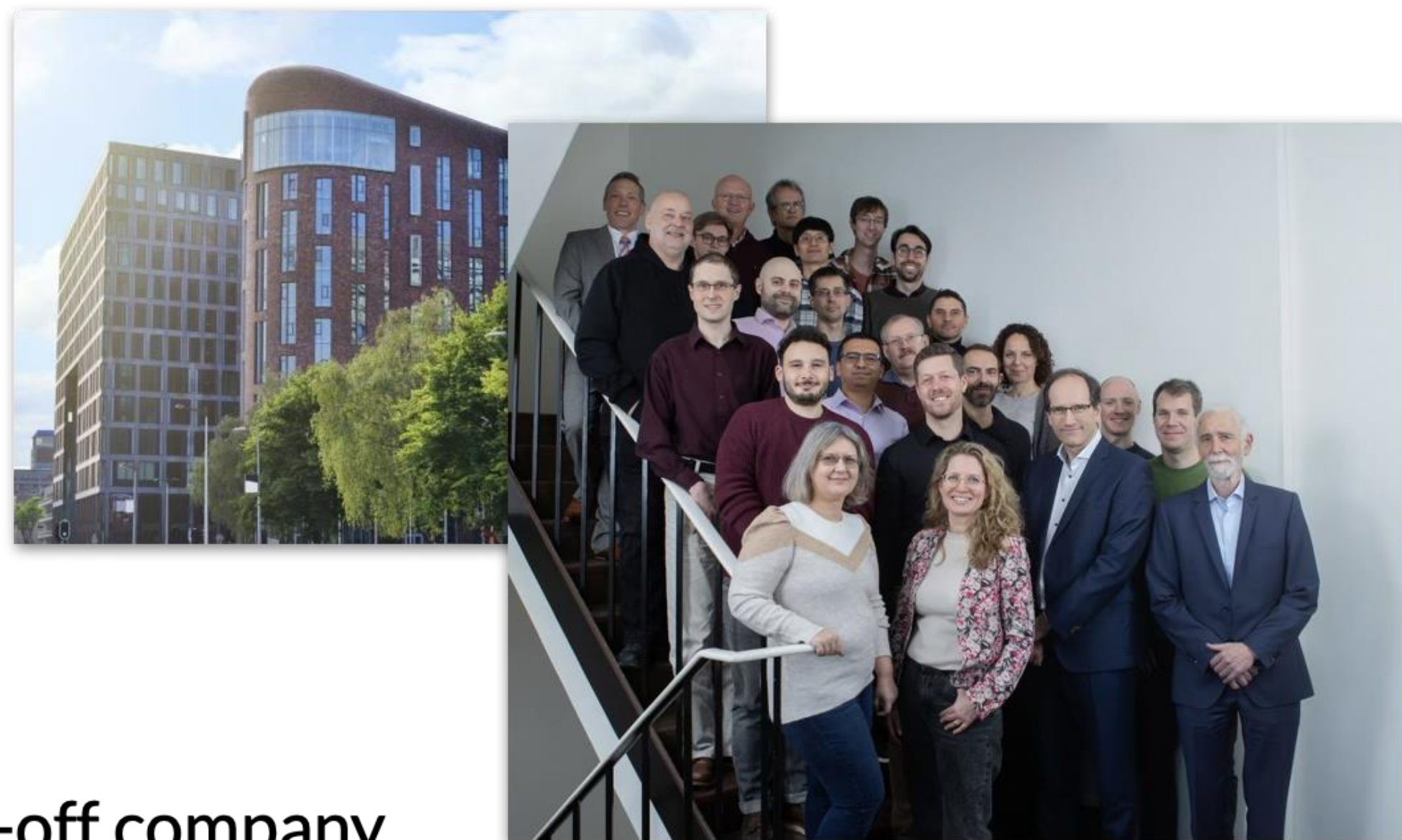
Introduction

Identify where you best fit



...and I use AMS

Software for Chemistry & Materials



Baerends@VU & Ziegler@Calgary



SCM: Spin-off company
(VU Amsterdam)

1970s

2026

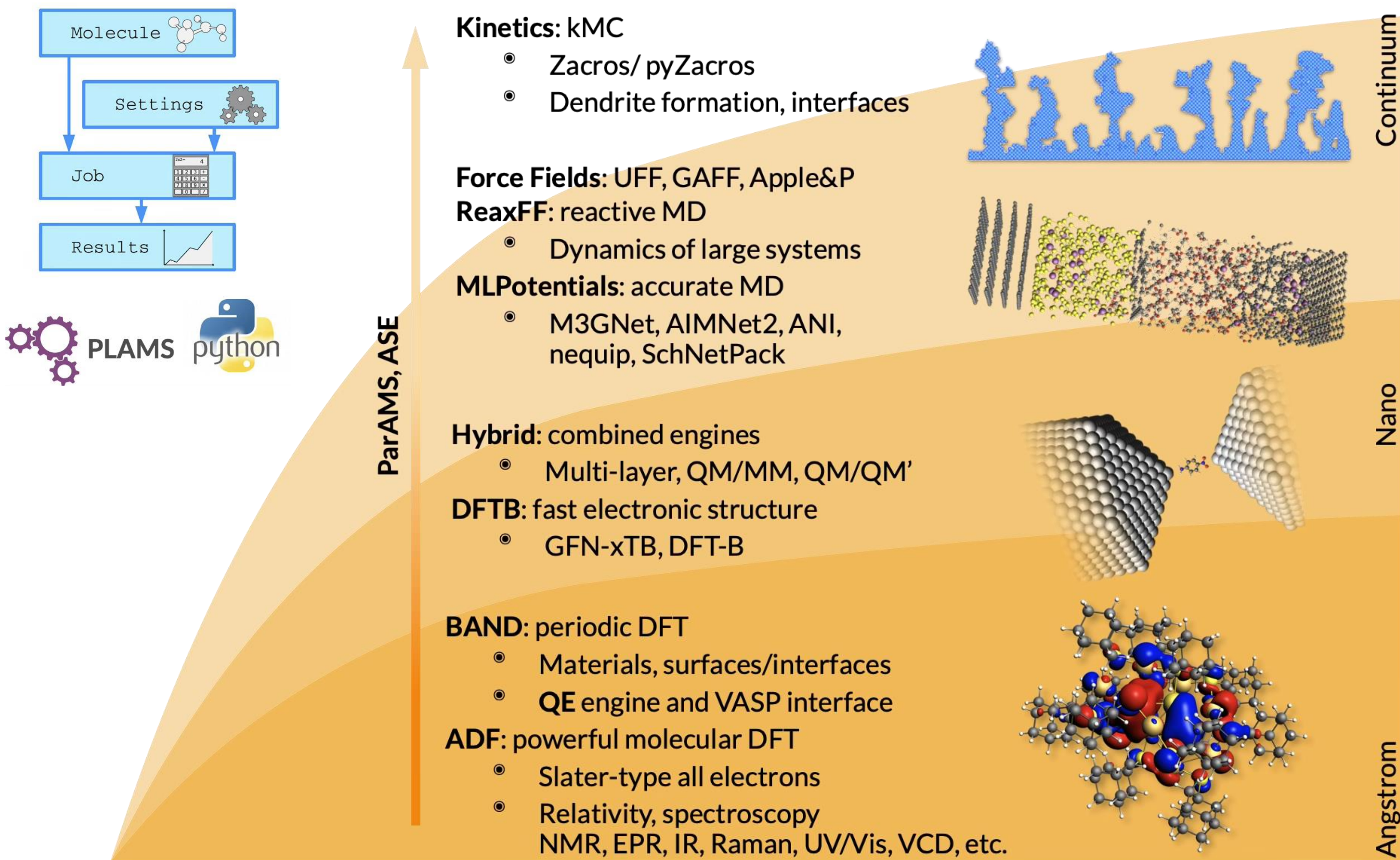
ADF = first DFT code for chemists
Study transition metal complexes
for catalysis

1995

Mitsui, Shell, Akzo, Unilever
Training in Amsterdam to optimize
catalysts

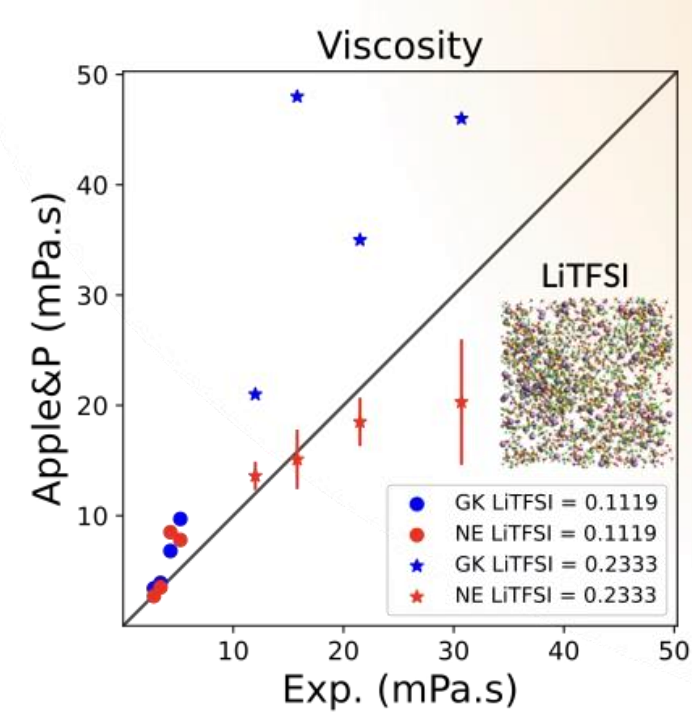
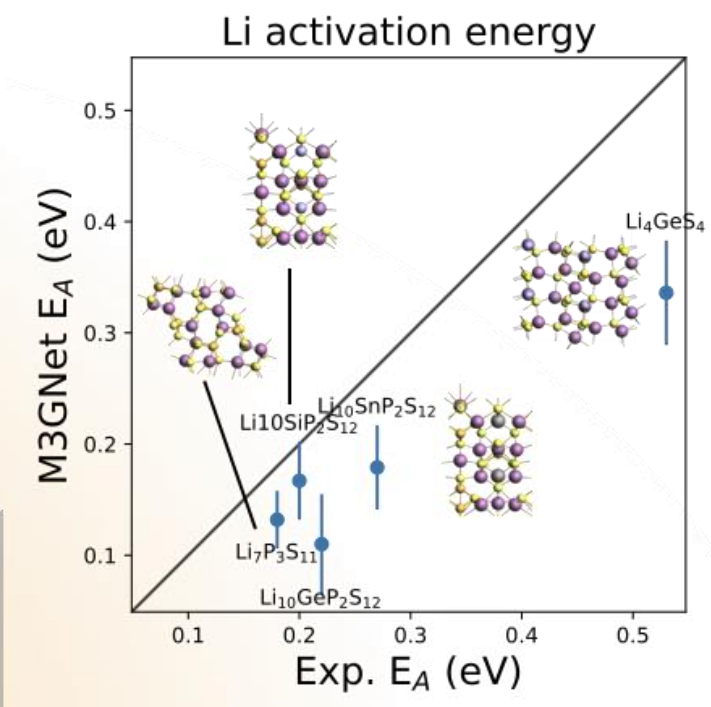
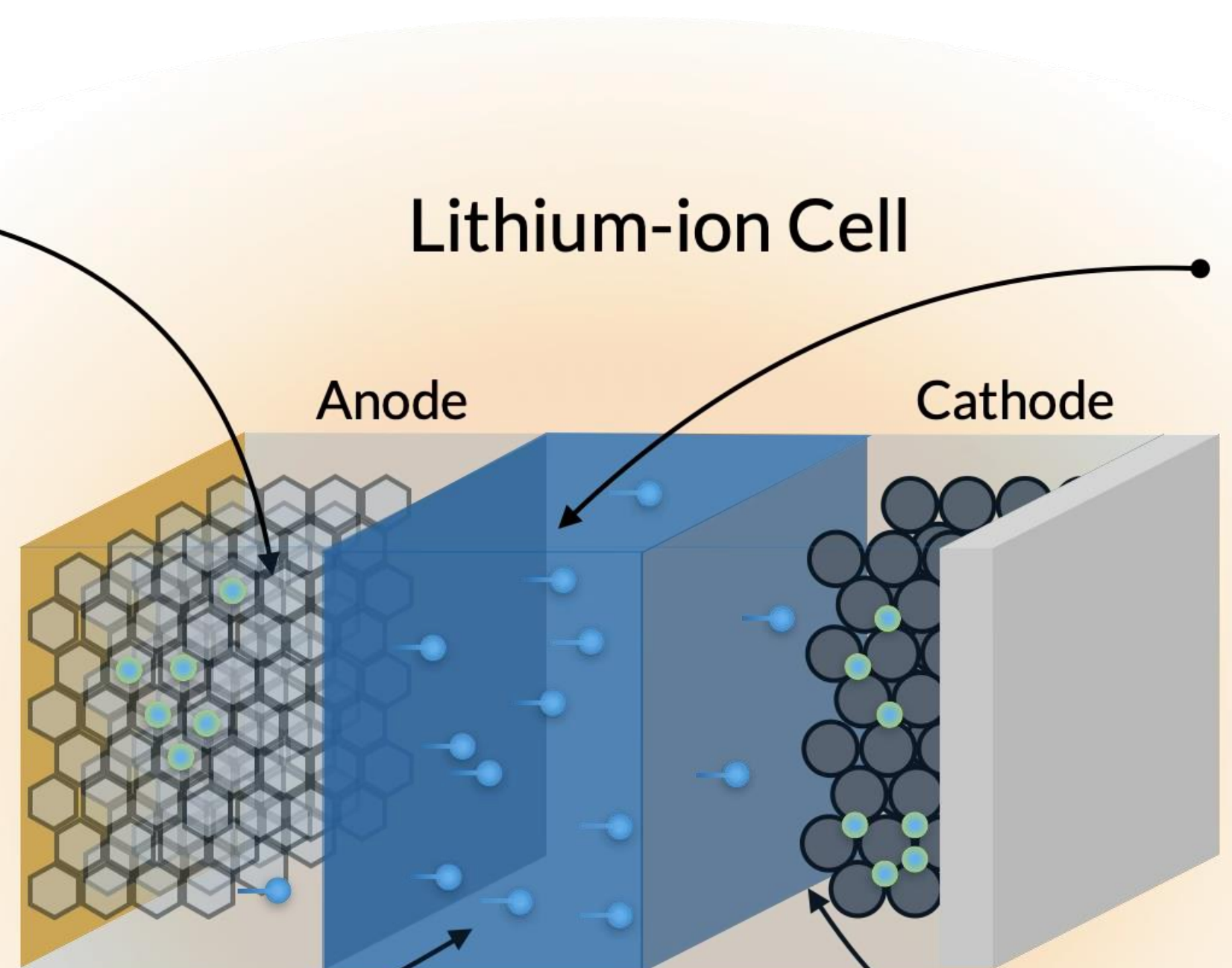
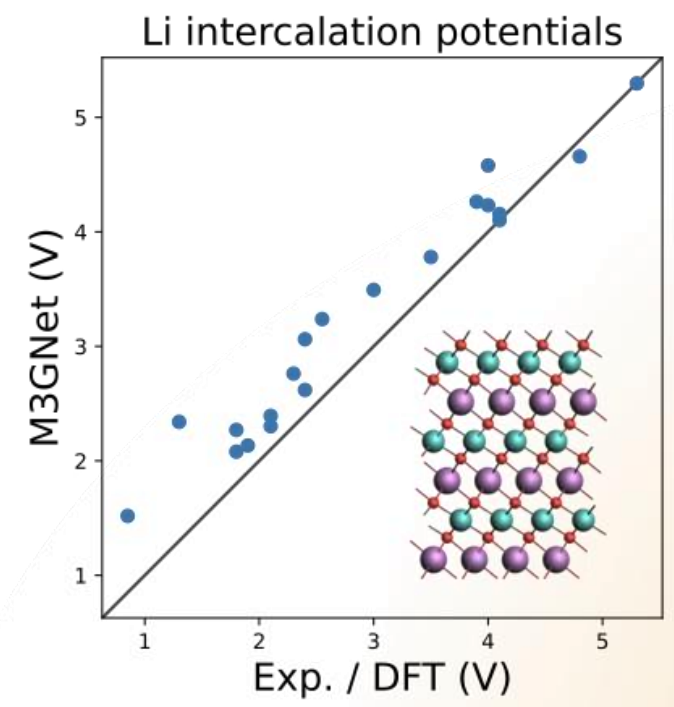
30 peoples (15 senior PhD's)
~ 15 developers
*Implement new features, debug,
optimize, docs & support*
+ Many academic collaborators

The Amsterdam Modeling Suite

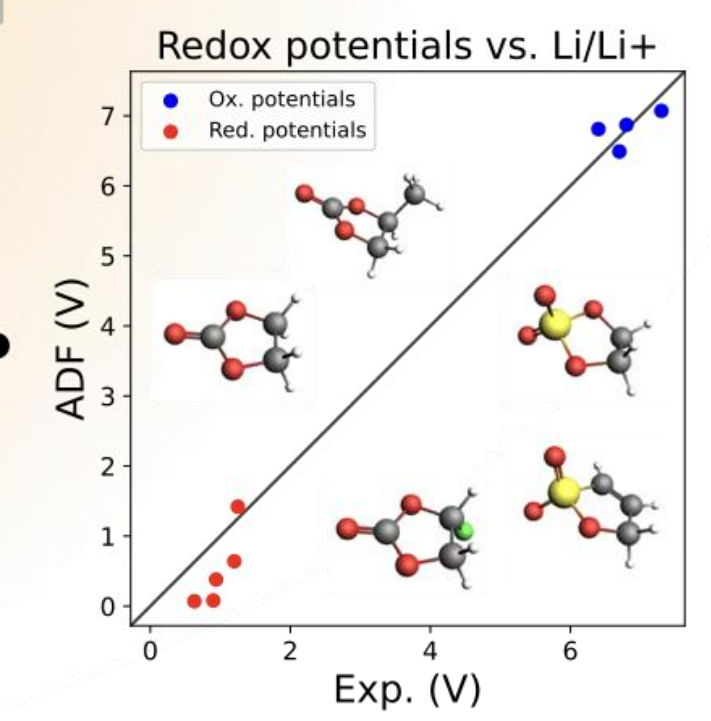


Batteries

Predict, optimize and design



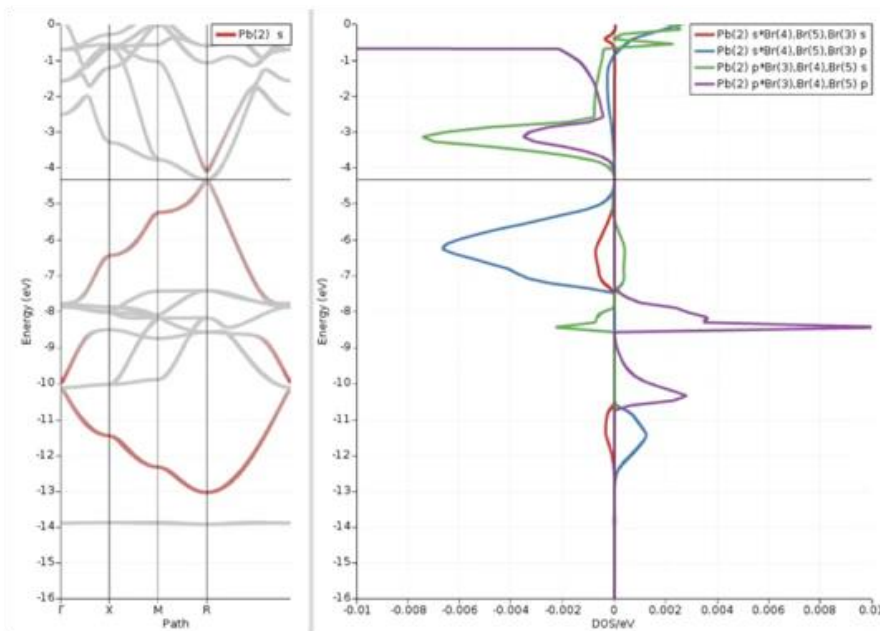
- ✓ Energy density: intercalation potentials, voltage profiles
- ✓ Kinetics: diffusion coefficients, activation energy
- ✓ Thermodynamics & stability: free energy path, redox potentials, viscosity



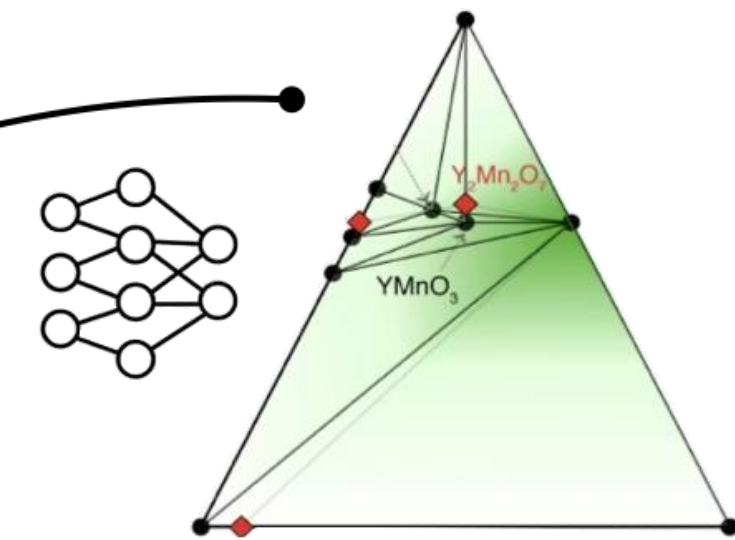
Semiconductors

Understand materials & processes

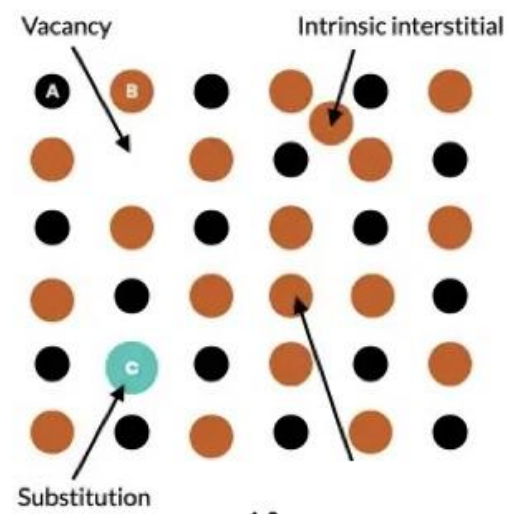
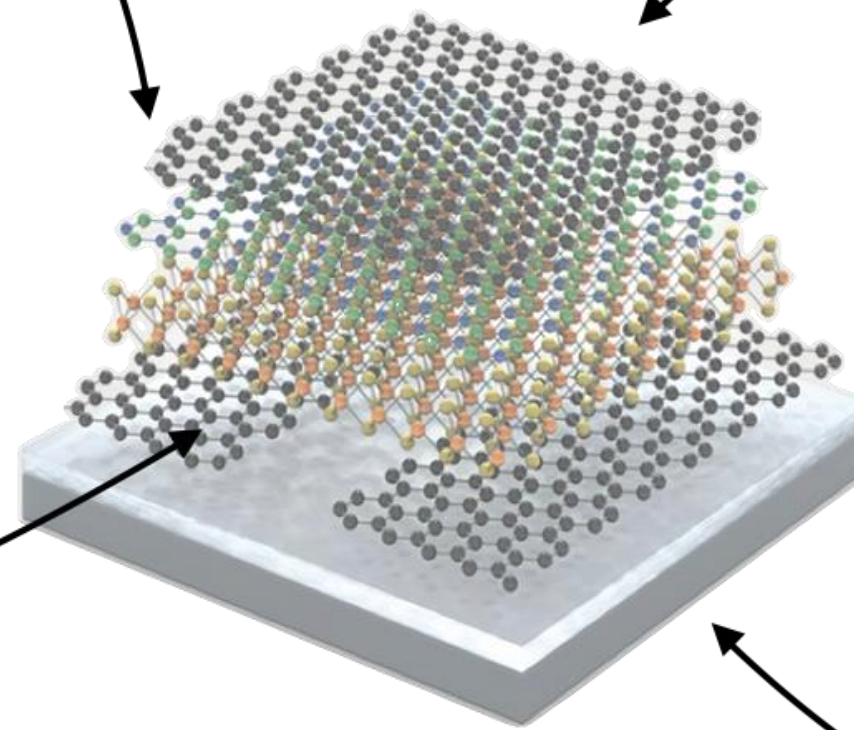
Electronic structure & spectroscopy



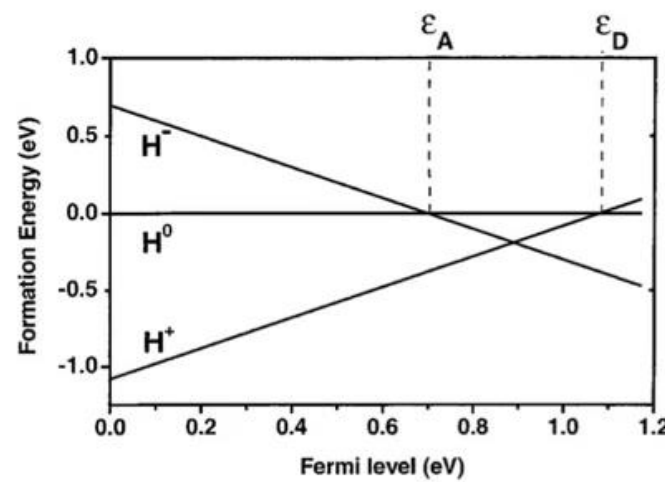
Compositional phase diagrams



Transistors and interconnects

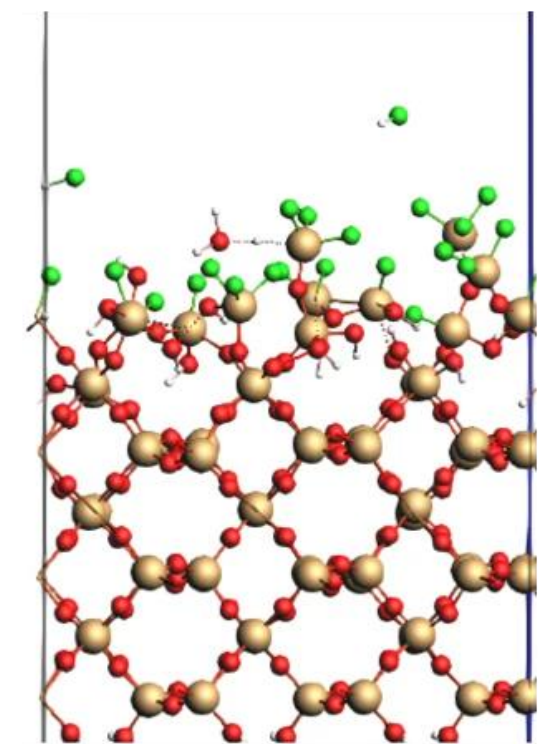


Defects



- ✓ Electronic properties: bandgaps, effective mass, mobility, phonons, defects, work function, etc.
- ✓ Materials optimization: phase diagrams
- ✓ Processes: deposition, etching, sputtering

Deposition & etching, reaction pathways



AMSjobs

The screenshot shows the AMSjobs GUI interface with several annotations:

- switch GUI module** and **Install packages**: Point to the **SCM** menu item.
- define & switch queues (remote queues)**: Points to the **Queue** menu item.
- reports & templates**: Points to the **Tools** menu item.
- job status**: Points to the status icons in the job list.
- change default, e.g. cores, nodes, walltime**: Points to the input fields in the queue configuration table.
- queue**: Points to the queue names in the table.
- see files for this job**: Points to the **Structures** and **Templates** folders in the left sidebar.
- job type**: Points to the colored buttons (ML, ADF, Hybrid, FF, DFTB, MOP) in the job list.
- search**: Points to the search bar at the bottom.
- all jobs / folder view**: Points to the view toggle buttons at the bottom right.

queue	cores	nodes	walltime	status
Sequential				⊘
Ivy	1			●
Sequential				●
Sequential				●
Ivy	1			●
Sequential				●
Sequential				●
Sequential				●
Sequential				●
Sequential				●

Now.. your turn!

www.scm.com/workshops/surf2026

Nicolas Onofrio, Software for Chemistry & Materials
onofrio@scm.com