Exploration of material properties : Interactive approach at the atomic scale

Okhotnikov Kirill

CEMHTI, CNRS.

CaSciModOT, 2013

The ExaViz project.

- **Marc Baaden, Laboratoire de Biochimie Théorique UPR 9080 CNRS / UNIVERSITÉ PARIS 7**
- B. Raffin, INRIA/MOAIS: Multi-programmation et Ordonnancement sur ressources distribuées pour les Applications Interactives de Simulation
- S. Robert, E. Melin, S. Limet, A. Turki, Laboratoire d'Informatique Fondamentale d'Orléans (LIFO), Université d'Orléans
- S. Cadars, CEMHTI Orléans
- N. Férey, LIMSI, Orsay

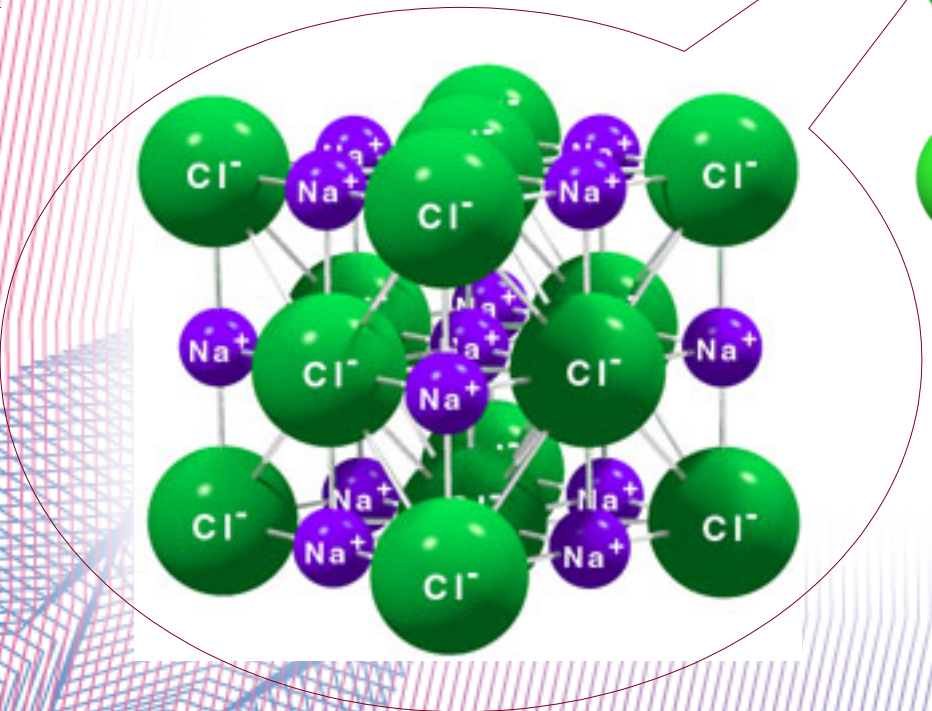
AGENCE NATIONALE DE LA RECHERCHE ANR

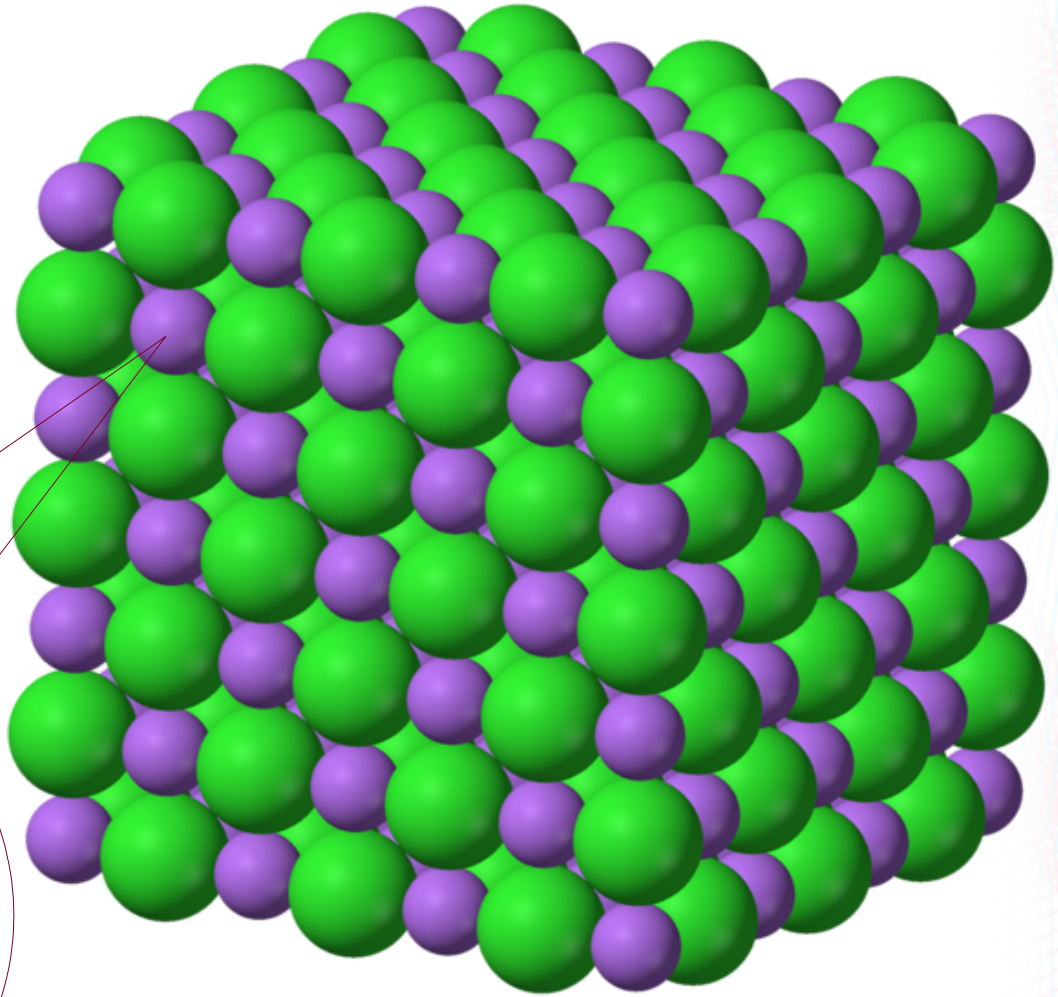
cnrs

UNIVERSITE D'ORLEANS

Crystal structure

- Periodicity.
- Unit cell.
- Atom positions.
- Symmetry.

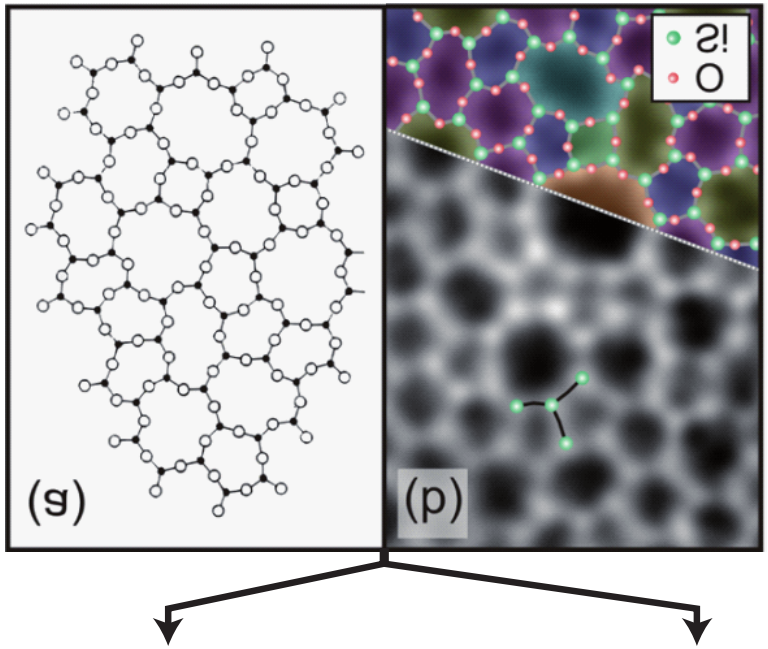




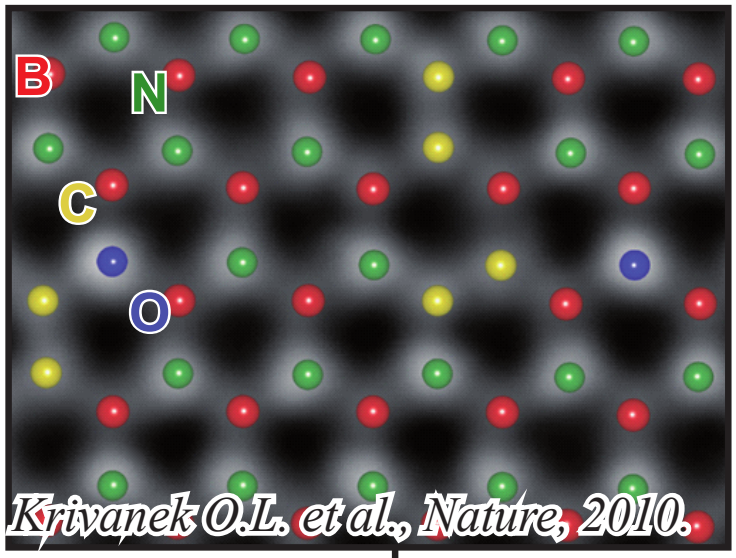
NaCl, $a=b=c=5.6402$ Å

Disorder in 2D objects.

2D SiO_2 "glass" on graphene sheet



O,C-doped (graphene-like) BN sheet



angles & distances

ring structures, building units & coordination sequences

atomic substitutions & compositional variability

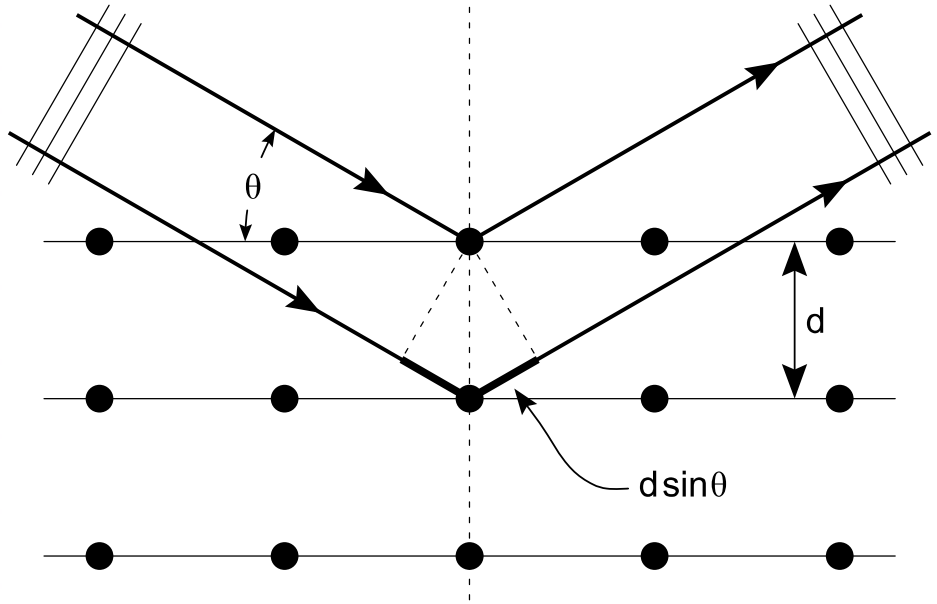
a) Zachariasen W.H., J. Am. Chem. Soc., 1932.

b) Lichtenstein L. et al., J. Phys. Chem. C, 2012.

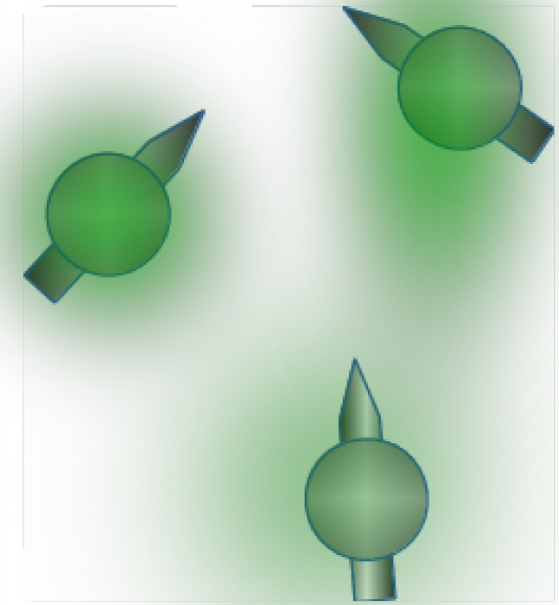
Disordered materials

- Metallic alloys: steel (Fe + C), bronze (Cu + Sn), alloy steel (Fe + Cr, Cu, Ni, Mo).
- Semiconductors: *n*-type (Si + P), *p*-type (Si + B).
- Superconductors: Nb+Ti1, $YBaCu_3O_{7-x}$
- Glasses and many-many more...

Experiment:
Diffraction vs NMR



Average over many period of the structure.

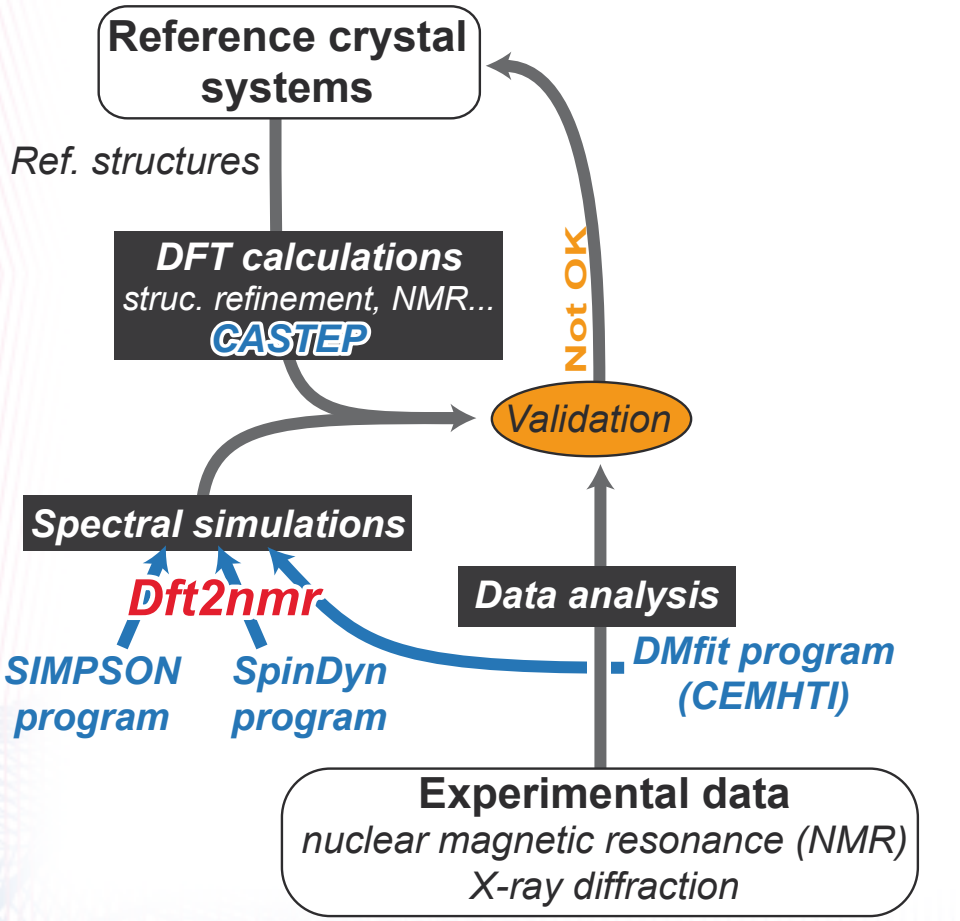


Sum of individual contribution of all local environments

Two different type of information!

Research work-flow

Molecular strutcures and properties of crystalline materials can be calculated with quantum mechanics *(eg, density functional theory, DFT: up to a few hundred atoms)*



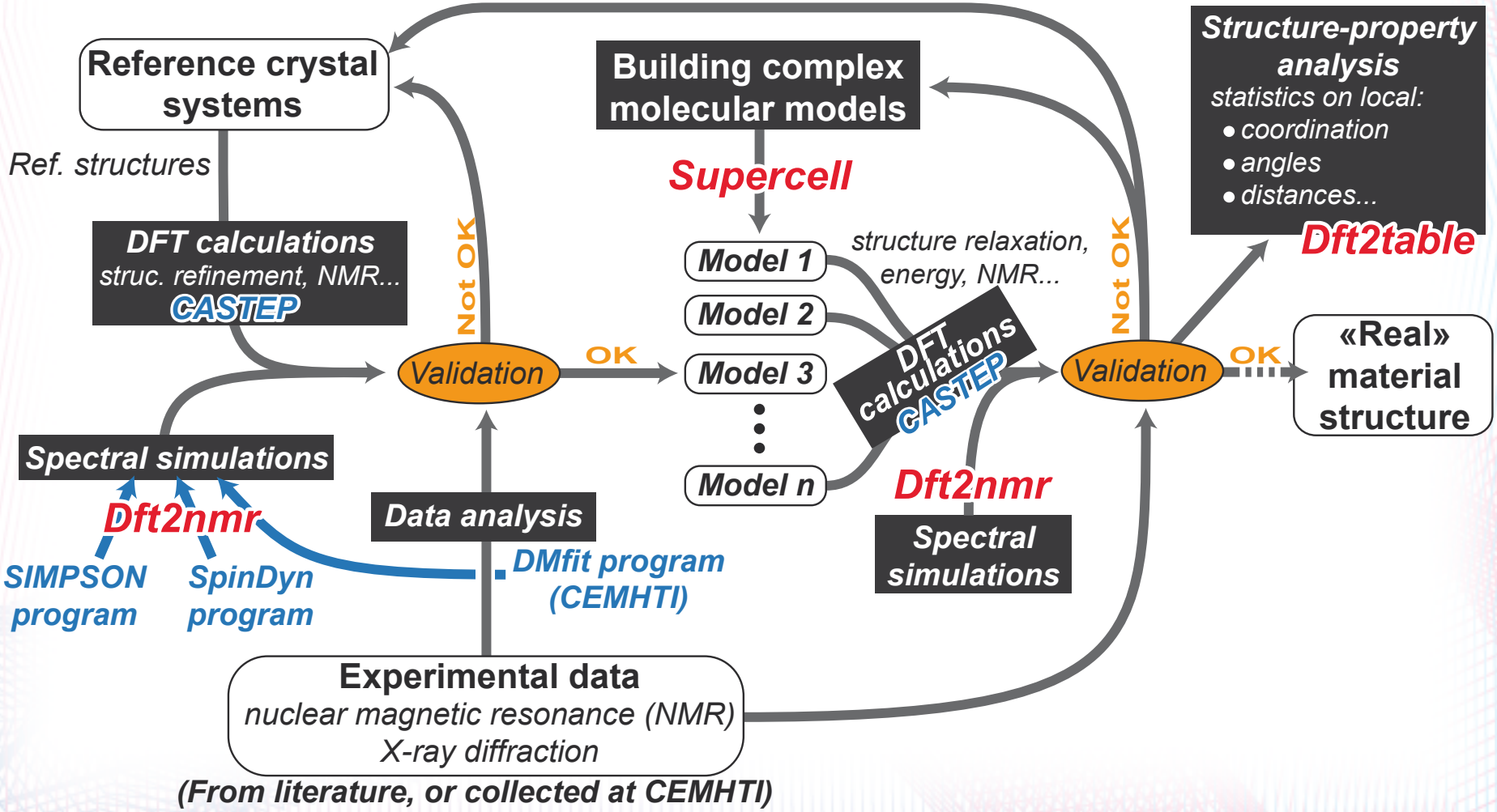
«Real» material structure

Existing program inter-operated with ExaviZ

Program developped within ExaviZ

Research work-flow

Molecular strutcures and properties of crystalline materials can be calculated with quantum mechanics *(eg, density functional theory, DFT: up to a few hundred atoms)*

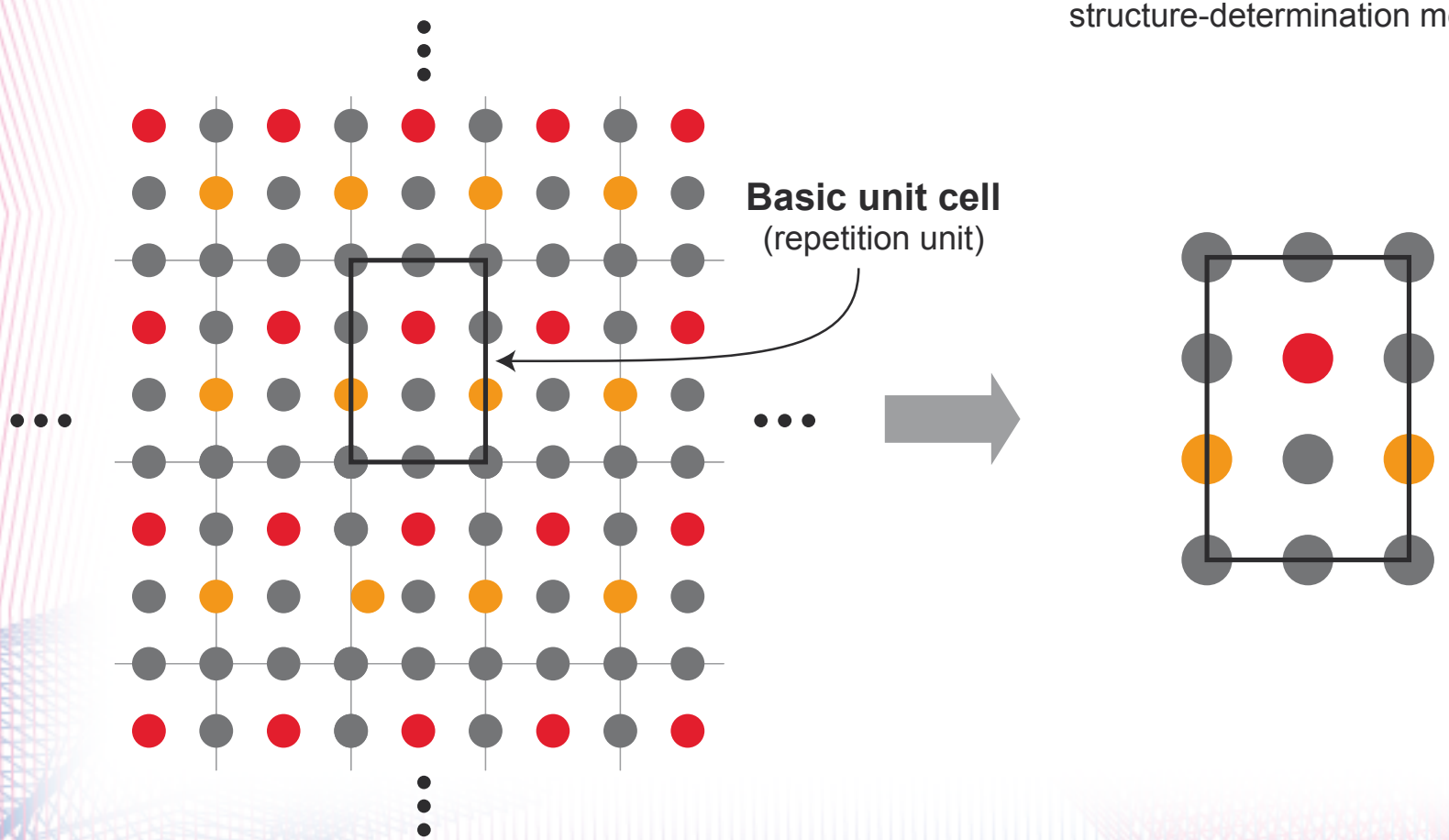


Structure averaging

The properties (optical, electronic, catalytic...) of many crystalline materials result from the presence of defects in their structures.

Real structure
= with real atoms (or vacancies)

Average structure
(as determined by classical crystal-structure-determination methods)

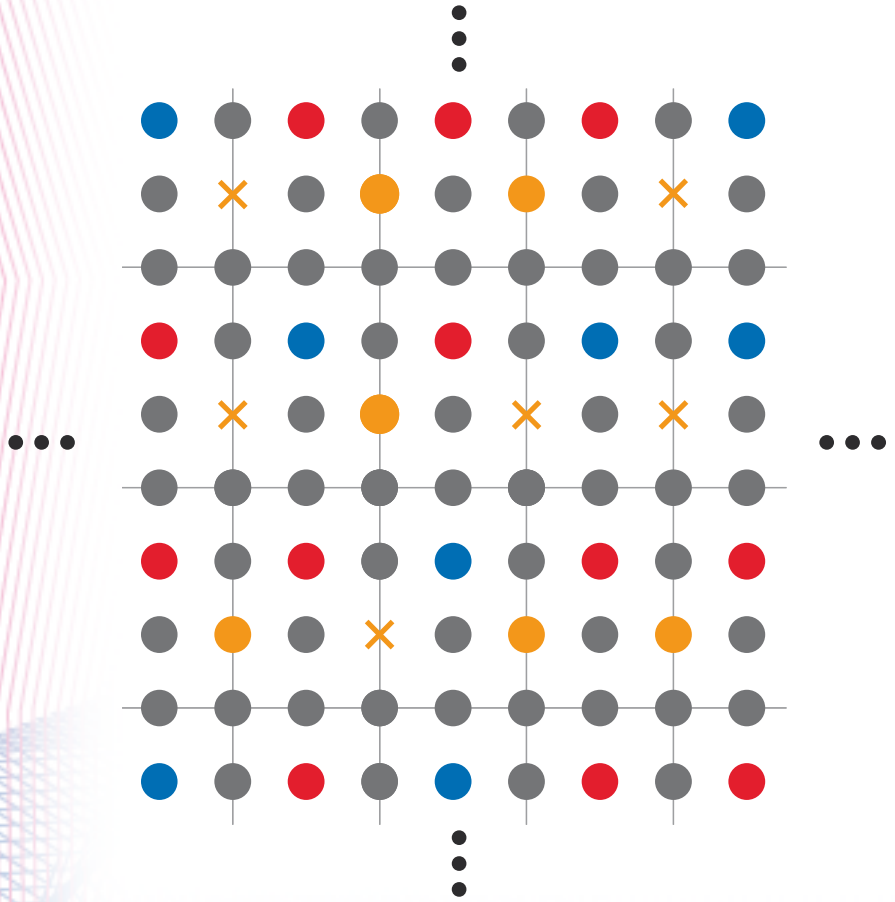


«Simple» crystal

Structure averaging

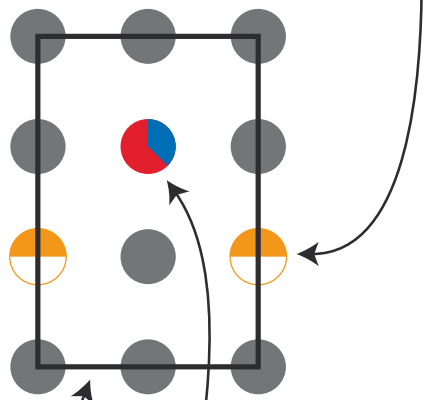
The properties (optical, electronic, catalytic...) of many crystalline materials result from the presence of defects in their structures.

Real structure
= with real atoms (or vacancies)



Random repartitions of ●, ●, ● and ×

Average structure
(as determined by classical crystal-structure-determination methods)



Fractional occupancy
only 50% of sites occupied by ● (others are vacancies)

Basic unit cell

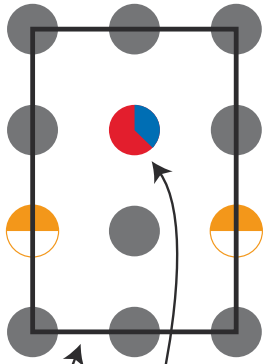
Mixed composition
site occupied at:
- 67% by : ●
- 33% by : ●

«Complex» crystal with atomic substitutions and vacancies

Supercell: Disorder modeling in crystals

The properties (optical, electronic, catalytic...) of many crystalline materials result from the presence of defects in their structures.

Average structure
(as determined by classical crystal-structure-determination methods)



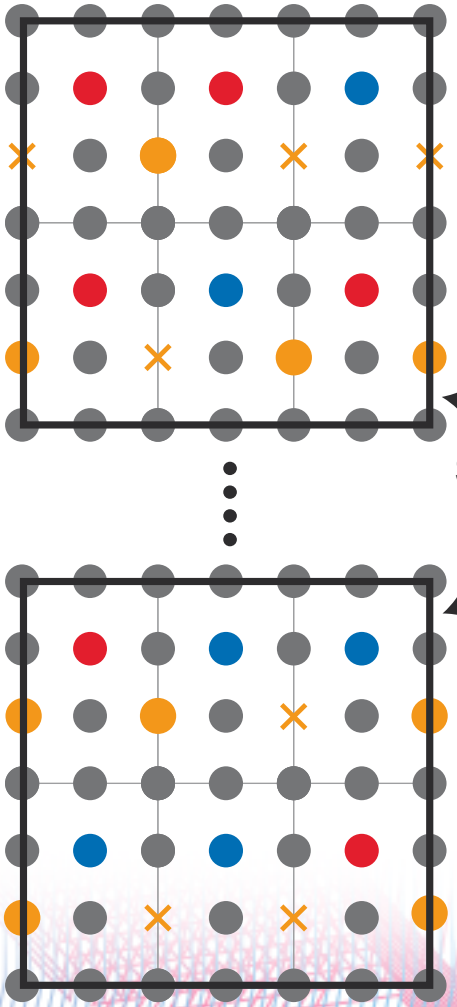
Basic unit cell

Supercell program
(open-source, to be released)

Fractional occupancy
only 50% of sites occupied by ● (others are vacancies)

Mixed composition
site occupied at:
- 67% by : ●
- 33% by : ●

Local structural models
with real atoms: necessary to predict local (eg, NMR) properties

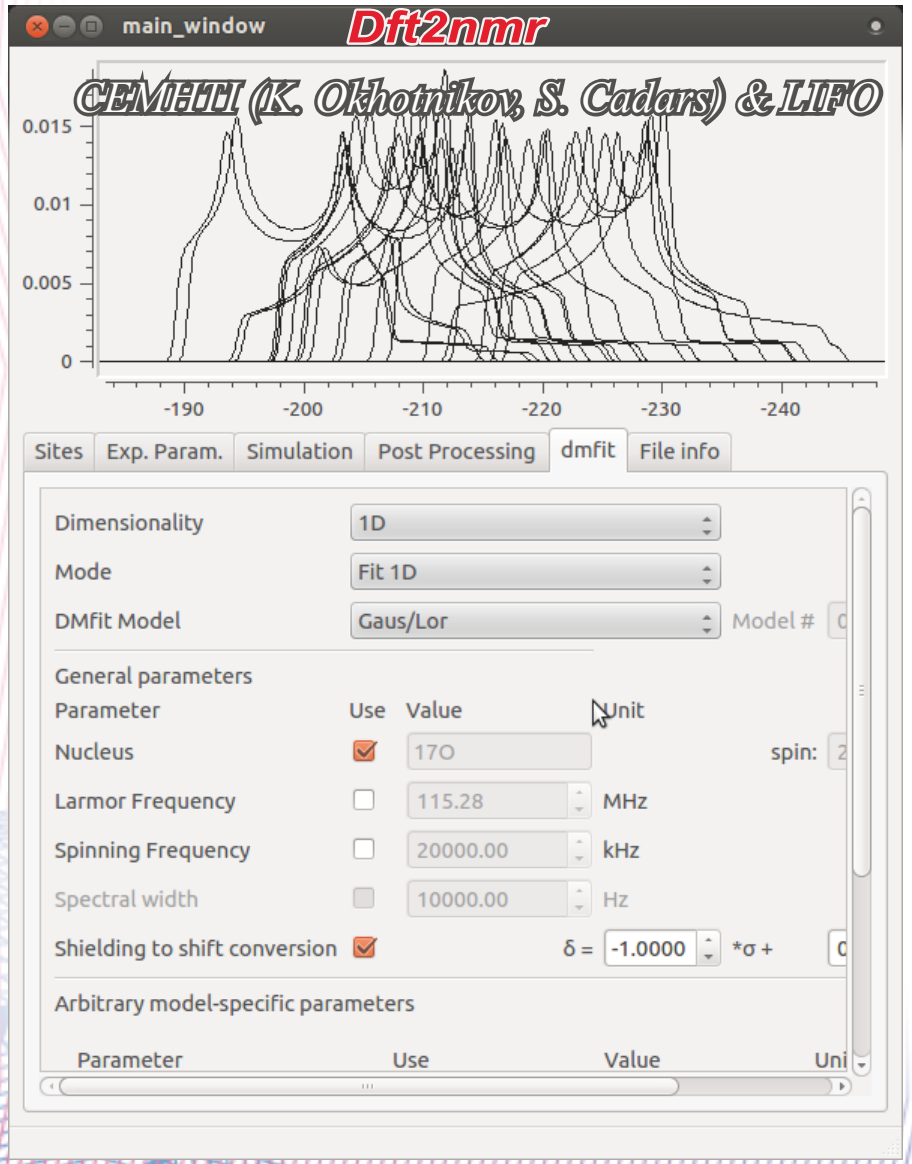


Supercell

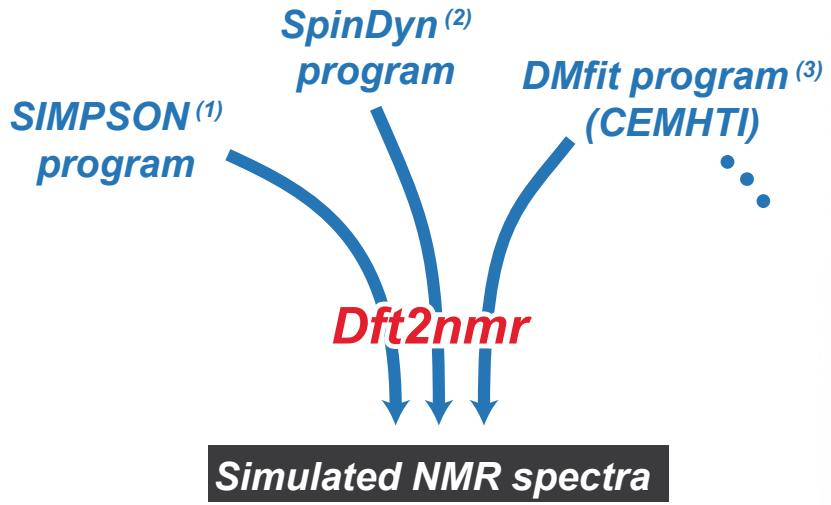
K. Okhotnikov, S. Cadars, Manuscript in preparation

DFT2NMR: Spectra simulation

Comparisons between experimental and calculated spectroscopic data require spectral simulations (*no existing user-friendly interactive tool for NMR data*).



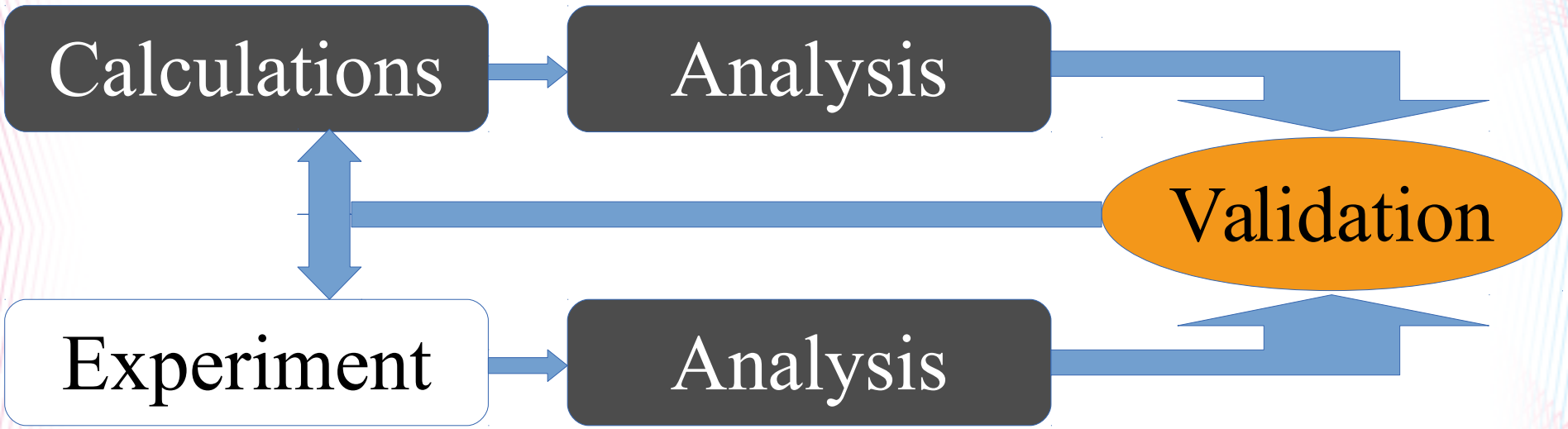
Integration of existing simulation tools



(1) M. Bak et al., J. Magn. Reson., 2000, 147, 296-330.
(2) Stevensson B. et al. J. Chem. Phys. 2011, 134, 124104.
(3) D. Massiot et al. Magn. Reson. Chem., 2002, 40, 70-76.

Research flow

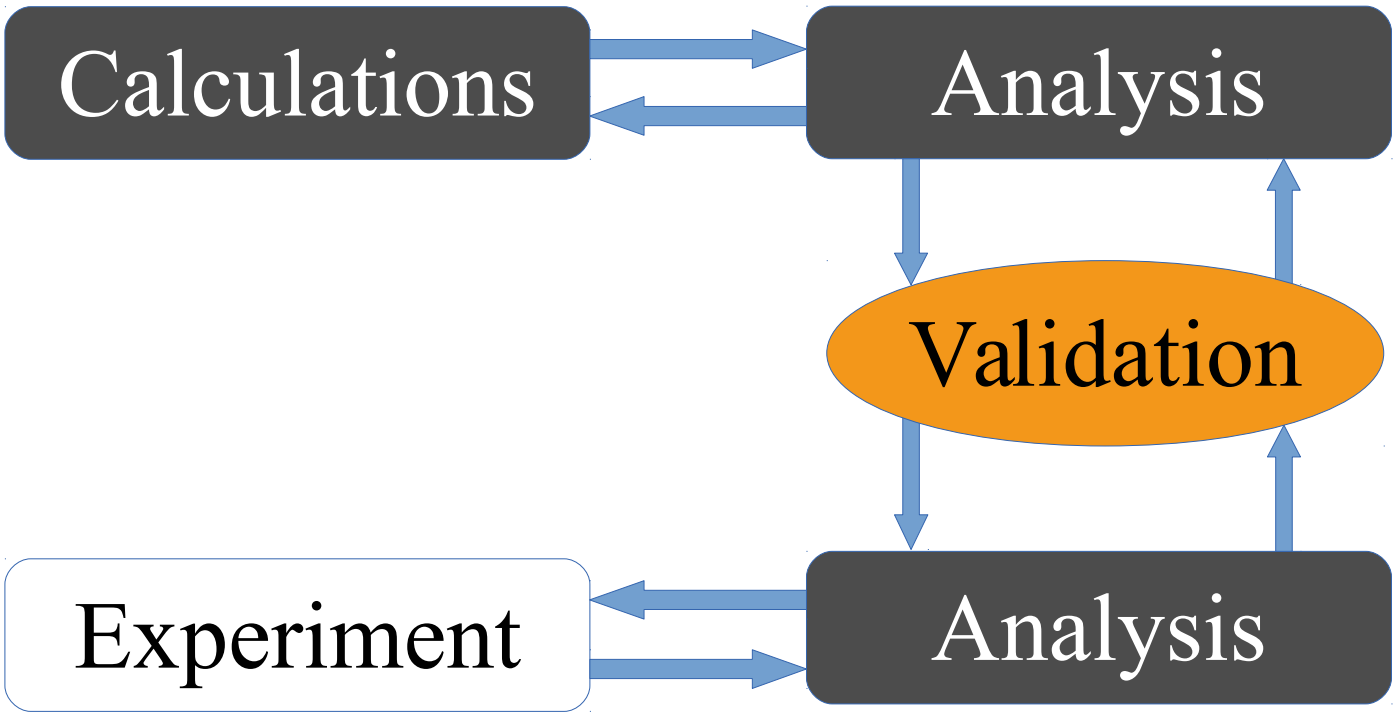
Standard



- Validation after full analysis.
- Permanent condition during simulation.

Research flow

Interactive



- Validation during analysis.
- Change condition during simulation.

FlowVR library (INRA-LIFO)

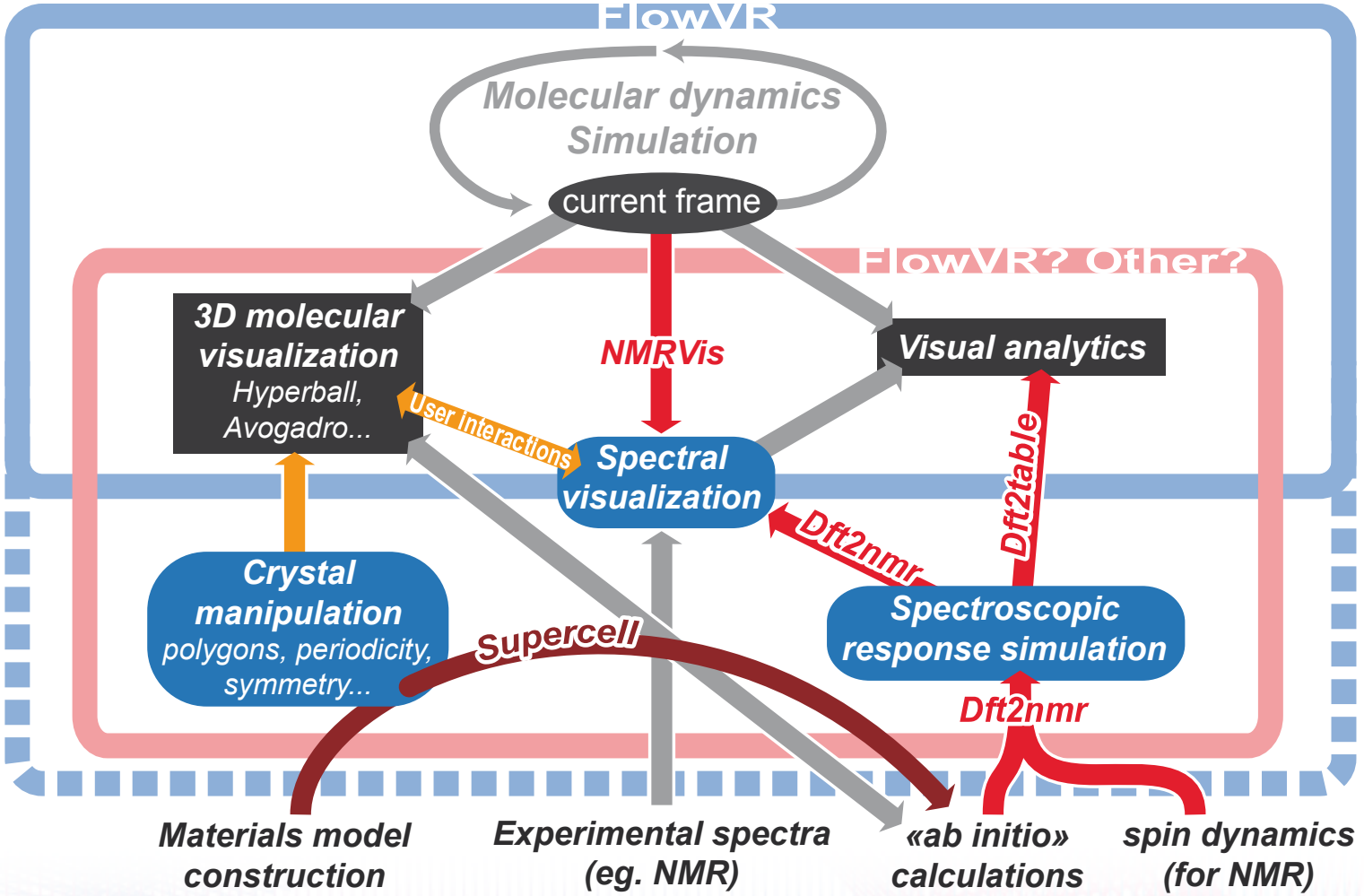
- Fast
- Flexible
- Universal
- Work over network

Modules Exaviz

- Calculations: MD Gromacs
- Visualization: OpenGL, CAVE, Qt
- Analysis: NMR spectra, Diffusion etc.
- Interaction: CAVE, Qt

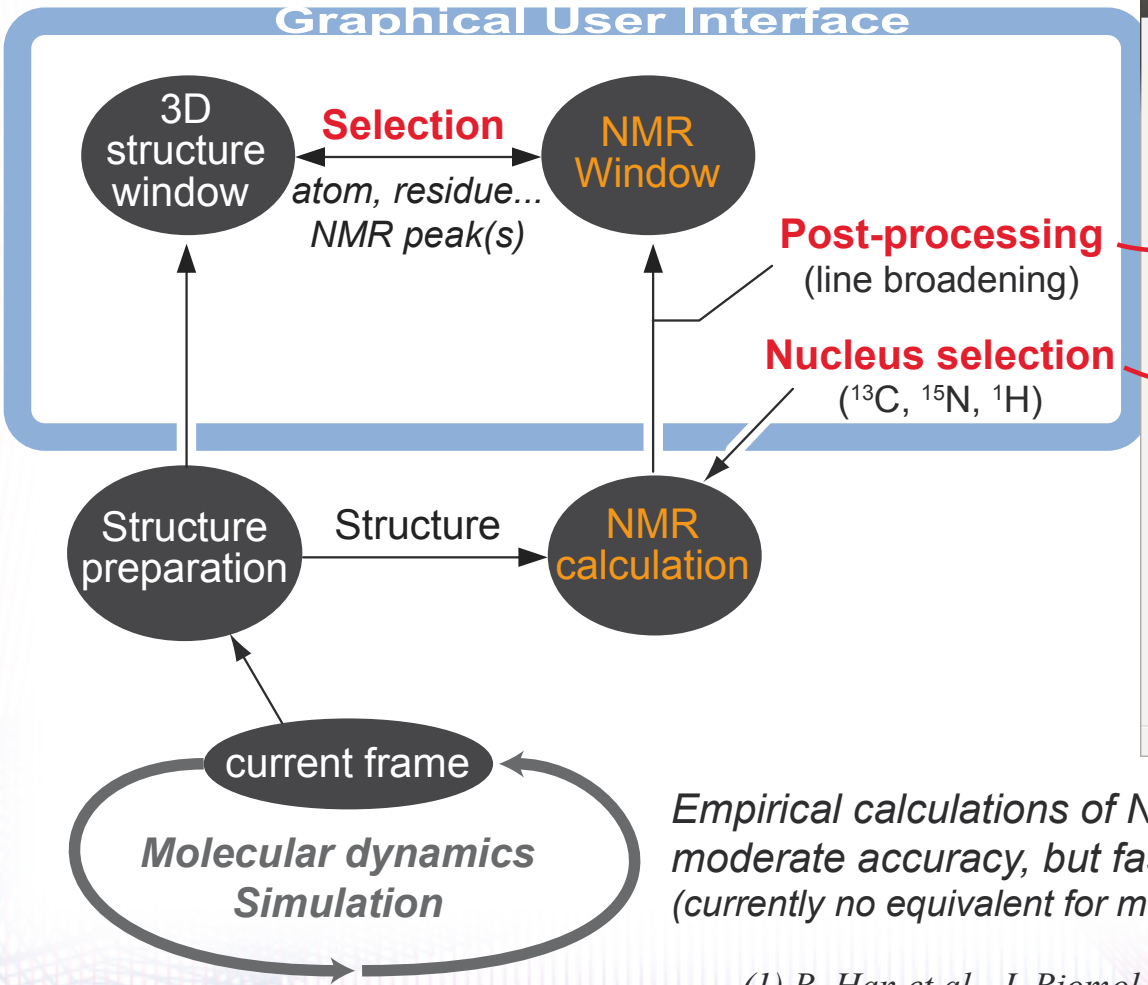
FlowVR + Material science

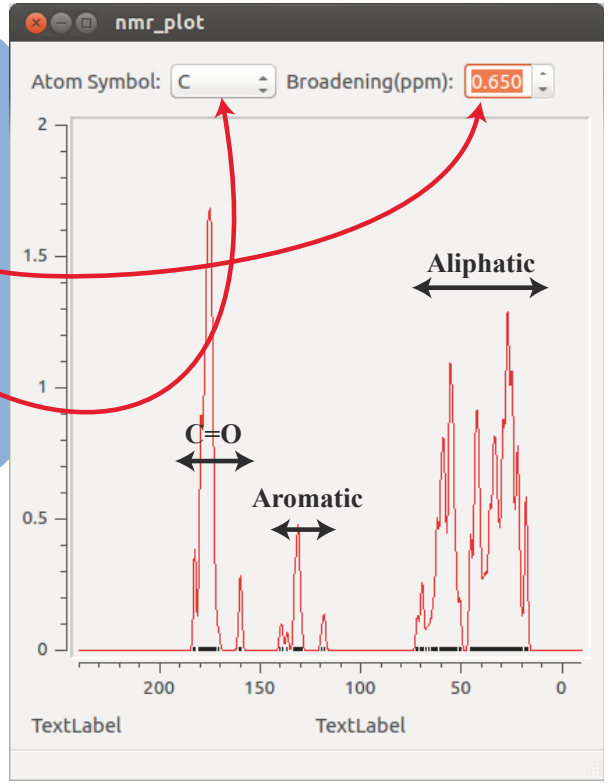
Spectroscopic data is central for the charcaterization of biomolecules or materials.
Tools are needed to **compare interactively experimental spectra & simulations**.



NMRVis modules (CEMHTI-LIFO).

A first prototype has been designed to **calculate and display NMR spectra « on-the-fly »** during **molecular dynamics simulations of biomolecules**.





*Empirical calculations of NMR properties (eg. **ShitfX2**[(1)])*
moderate accuracy, but fast (a few sec. for ca. 10^3 atoms)
(currently no equivalent for materials)

(1) B. Han et al., J. Biomol. NMR, 2011, 50, 43-57.

Conclusion and prospective.

Implemented.

- Software tools for building complex system: supercell, dft2nmr.
- NMR calculation and FlowVR visualization module was developed using statistical prediction approach.

In process

- Integration of the NMRVis module to ExaviZ workflow.
- Integration of *Ab-initio* NMR spectra calculation to ExaviZ.
- User interactions with spectra and molecules.
- Other physical properties implementation.

Thank you very
much for your attention.