EPFL

ChE-609

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Basics of machine learning for chemistry and materials science

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Why ML in chemistry and materials science?

- If we **agree** molecular simulation is useful:
  - Then: let's see where ML can help

The idea for a given *intermolecular potential* "*exactly*"
compute the *thermodynamic* and *transport* properties of
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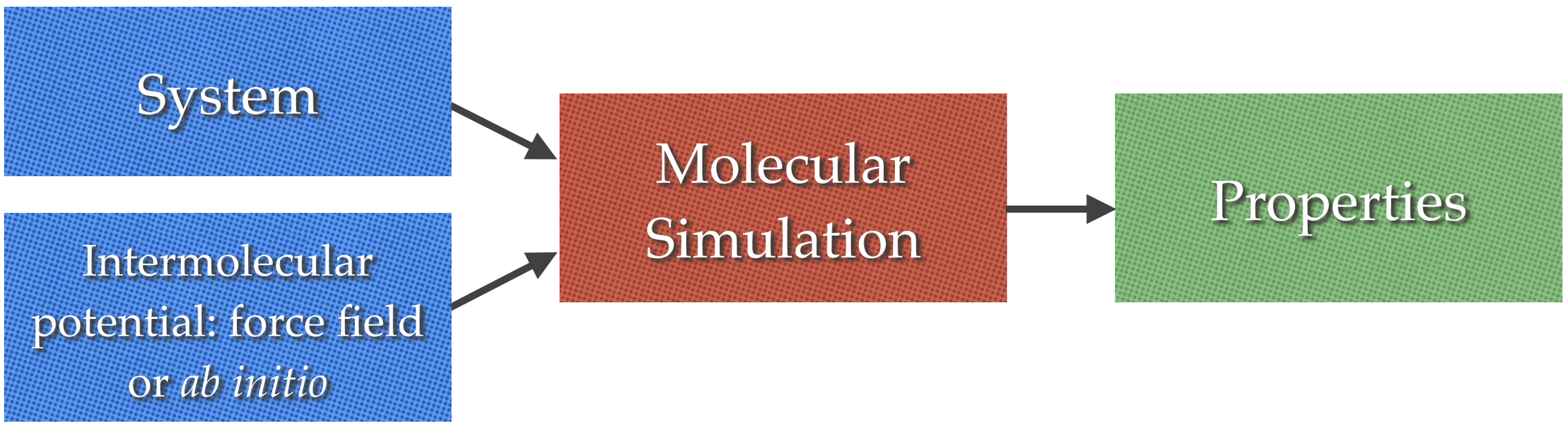

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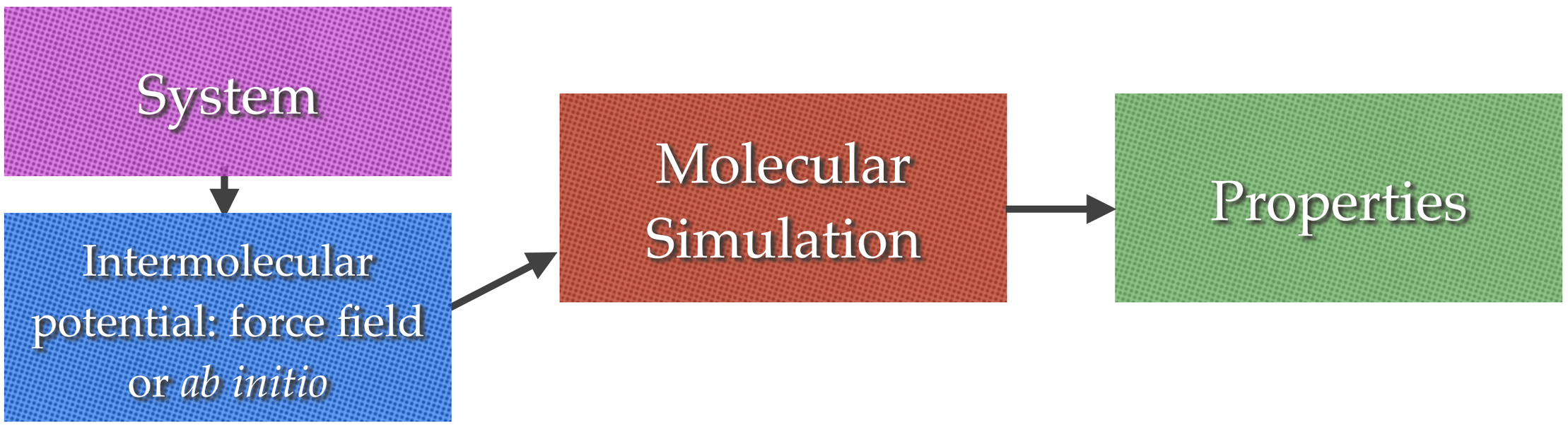

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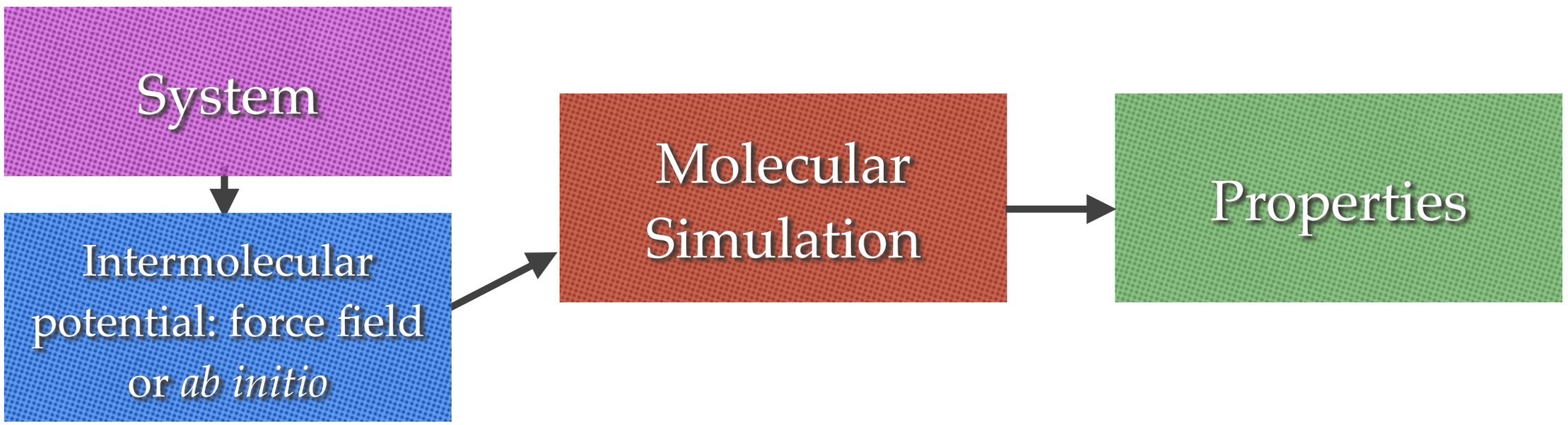

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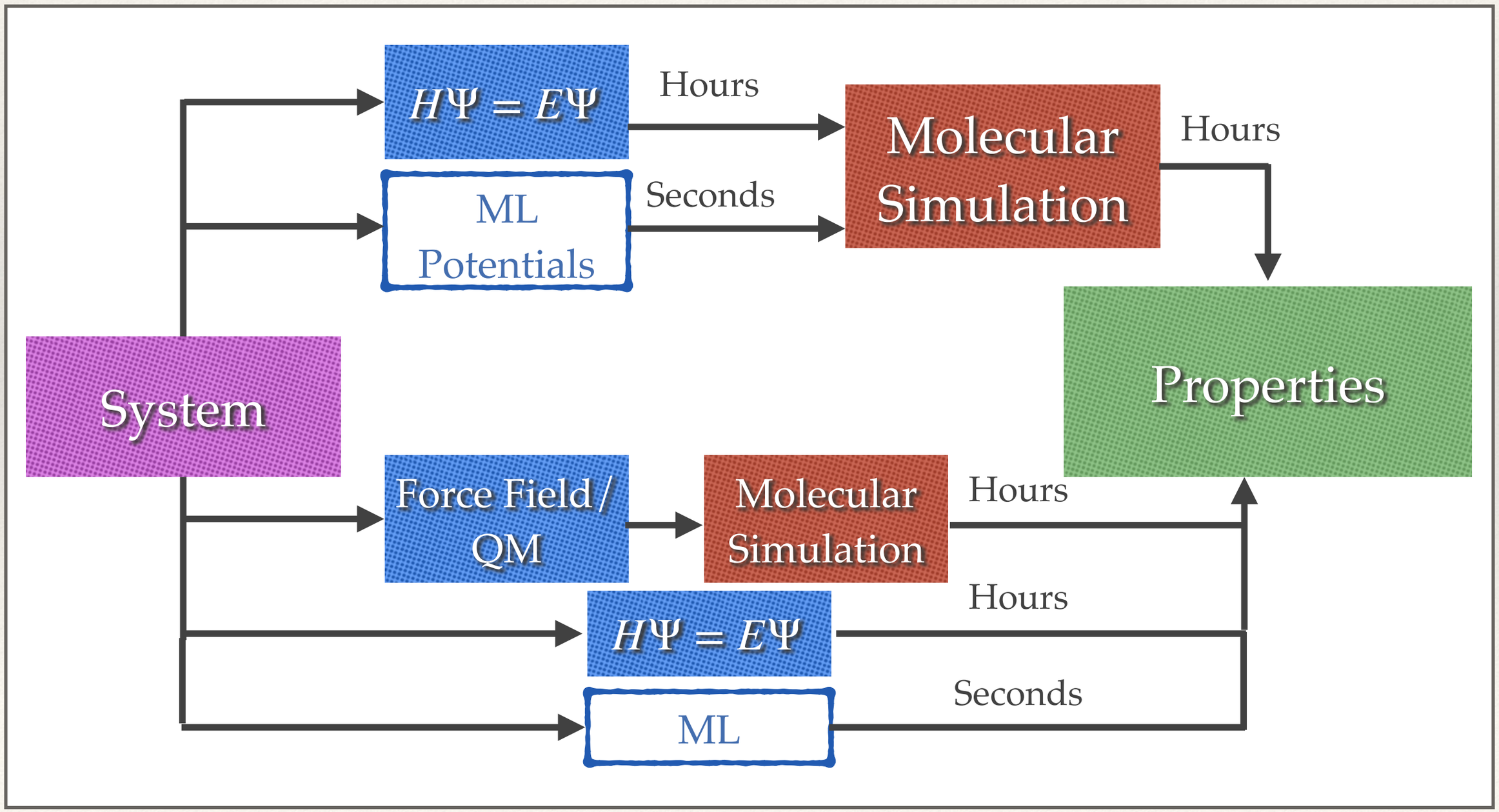

Why ML in chemistry and materials science?

- ML enables us to do new things too!

  - We have access to enormous amount of data

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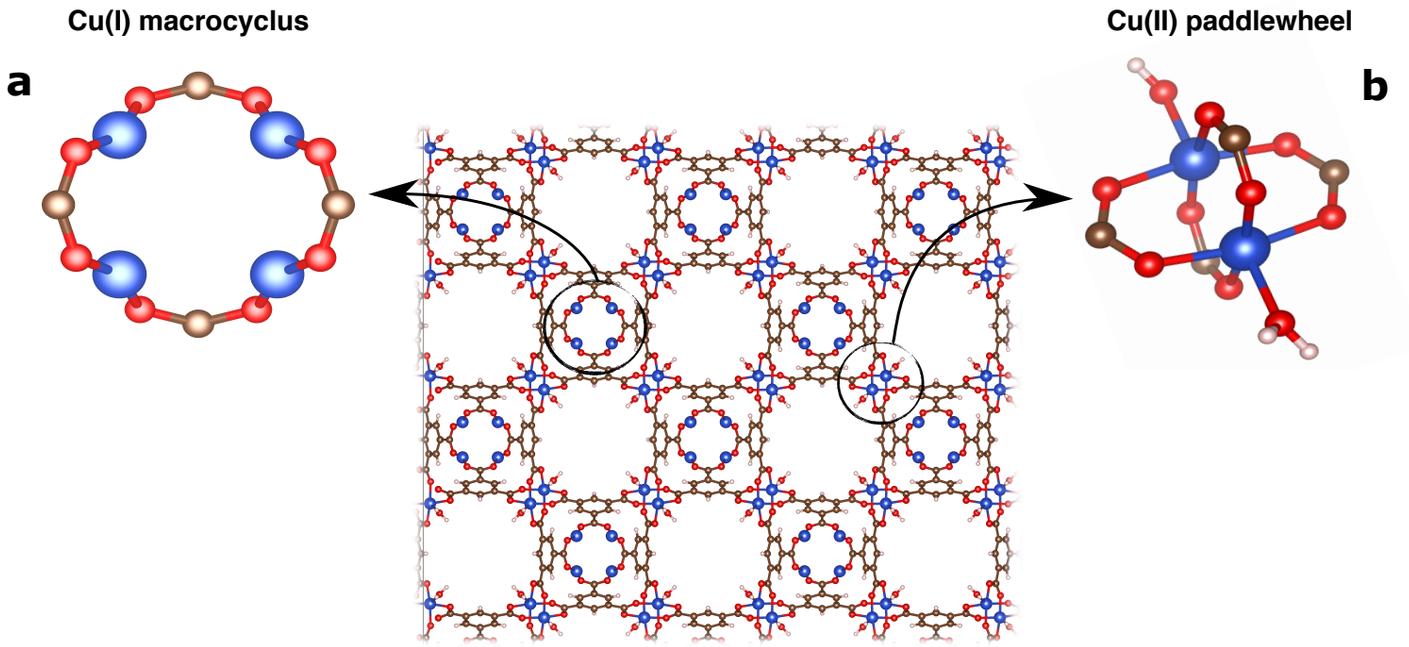
Oxidation states —> metal centres of MOFs



Current approaches

- Empirical assignment
- Theoretical models —> bond valence approach
- Quantum calculations/spectroscopy

Jablonka, et al. submitted (2020)

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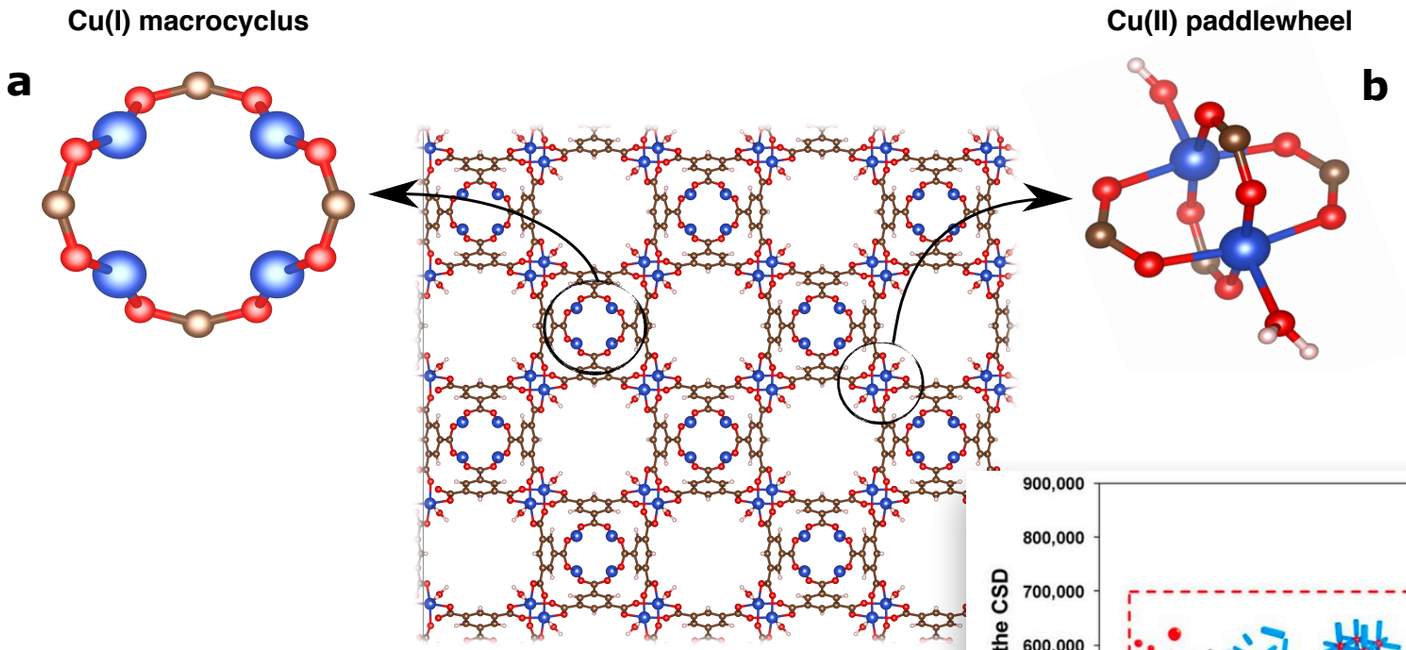

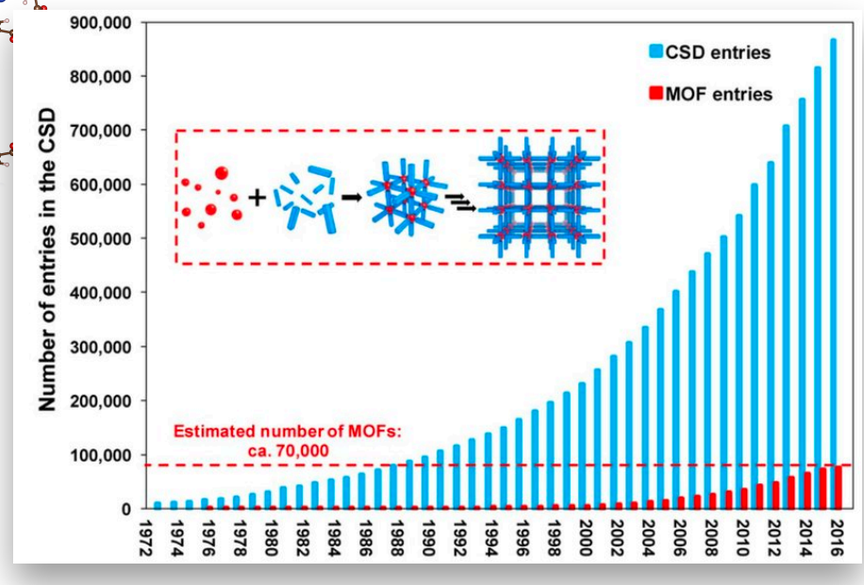

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Moghadam et al. Chemistry of Materials (2018)
Jablonka, et al. submitted (2020)

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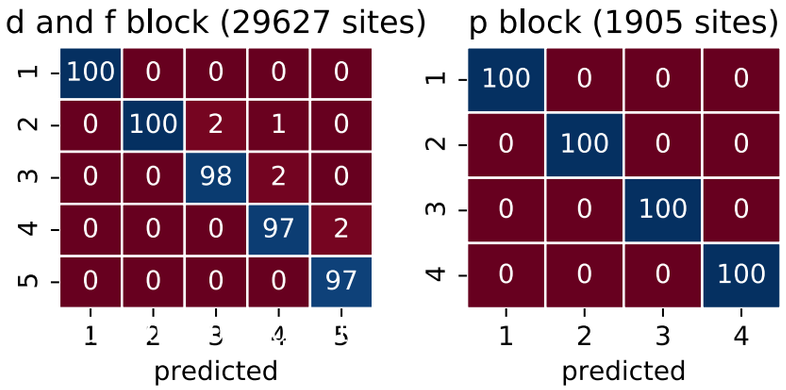

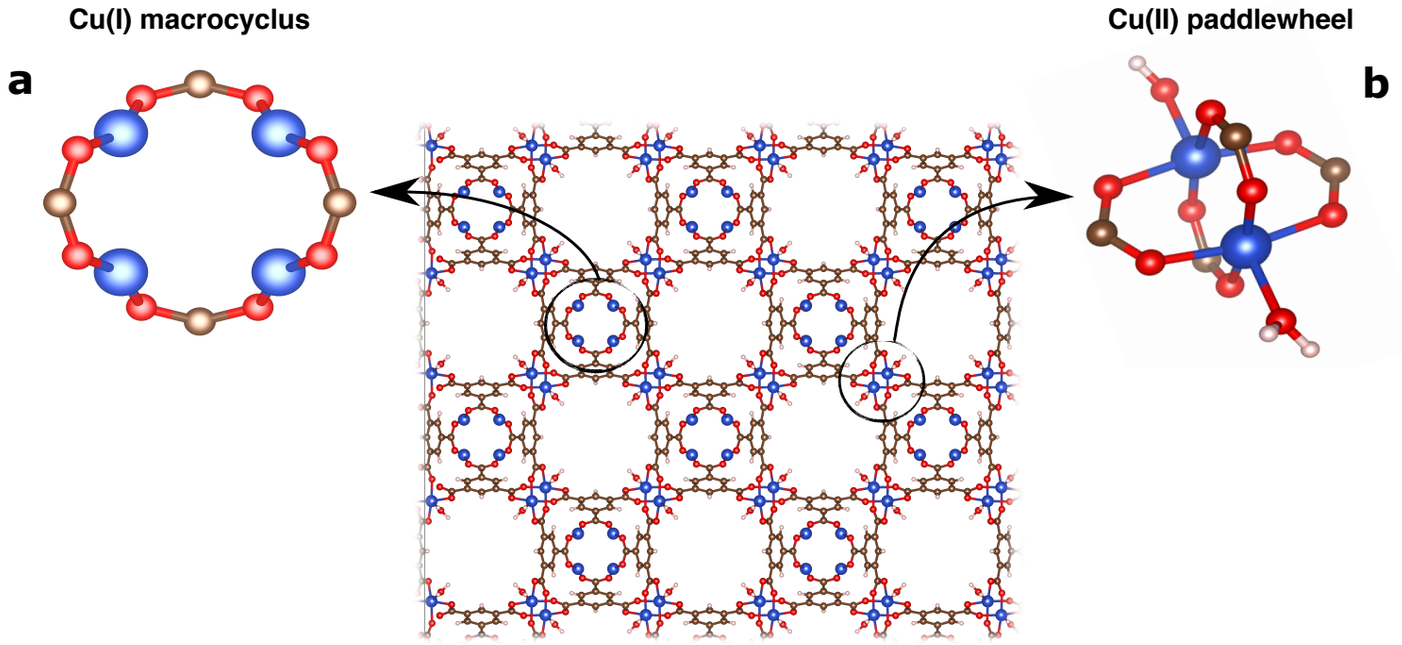

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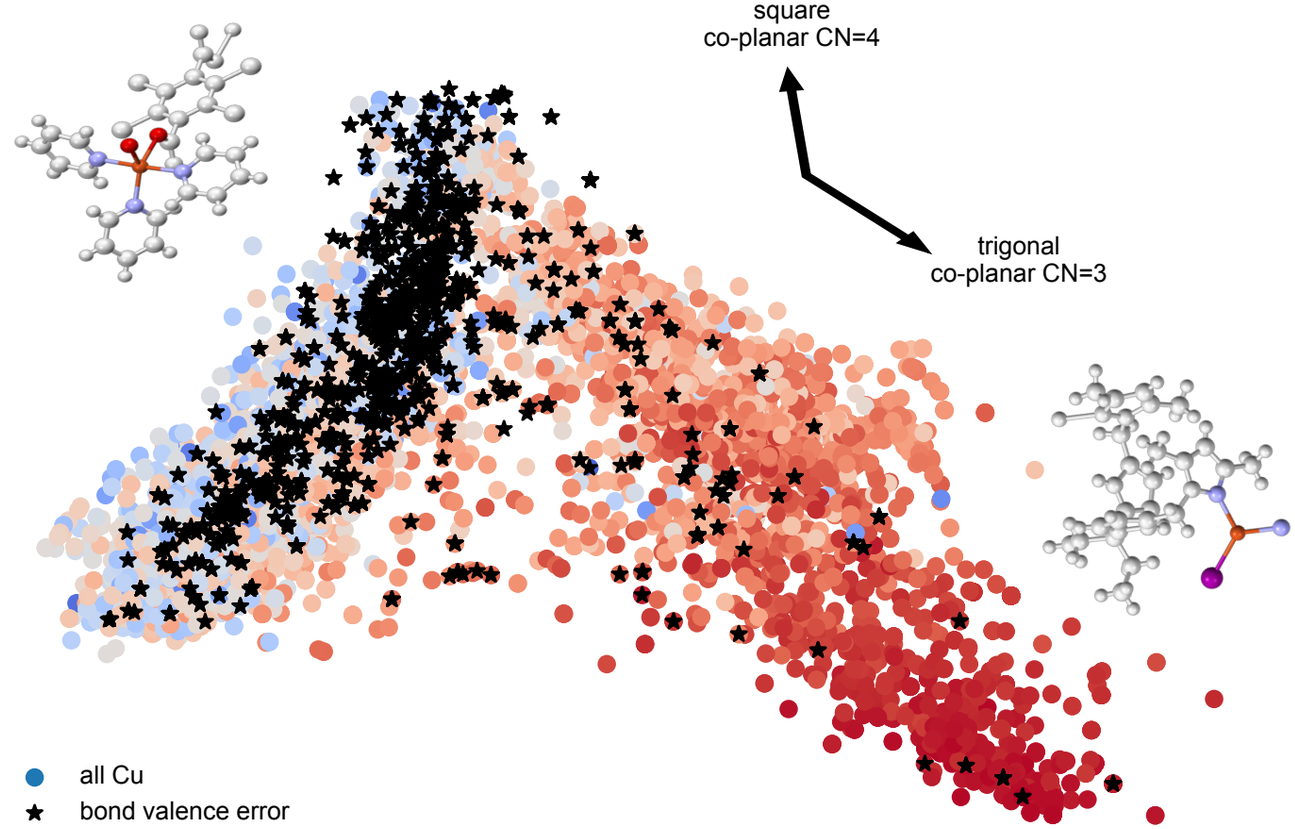

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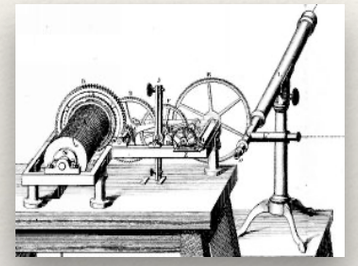
The “fourth paradigm” of science

1600 1950 2000

Empiral Science (1st Paradigm)



Experimental Observation

Theoretical Science (2nd Paradigm)

$$F = ma$$

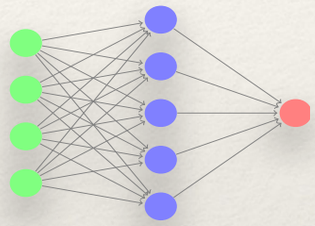
$$\hat{\mathcal{H}} |\psi\rangle = E |\psi\rangle$$

Development of Theories and Generalizations

Computational Science (3rd Paradigm)

Simulation of complex phenomena, High troughput computational screenings

Data Driven Science (4th Paradigm)



Machine Learning

“It is not that machines are going to replace chemists. It’s that the chemists who use machines will replace those that do not.”

- Derek Lowe, In the pipeline, Science Mag.

“AI is good at automatic tasks, rather than jobs.”

- Andrew Ng, Google Brain and Stanford