Machine Learning for Materials and Chemistry

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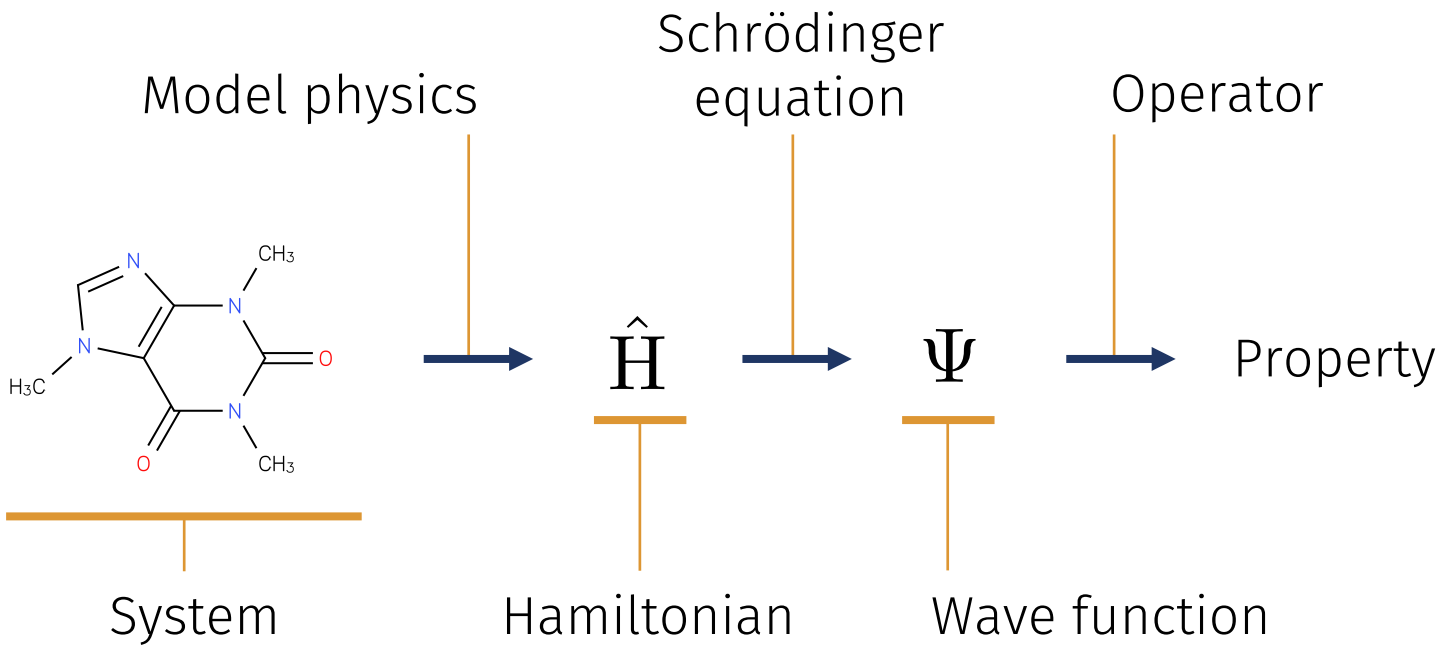
nablachem.org

Which problem do we try to solve?



Computational complexity

Depends on system size n

DFT	$O(n^3)$
HF	$O(n^4)$
MP2	$O(n^5)$
MP3	$O(n^6)$
MP4	$O(n^7)$
CCSD	$O(n^6)$
CCSD(T)	$O(n^7)$
CCSDT	$O(n^8)$
CCSDTQ	$O(n^{10})$
FCI	$O(n!)$

What is this course about?

Foundation of machine learning
Rules of the game

Representations
Mathematical model of molecules/materials?

Regression
Quantified prediction

Classification
Grouping, dimensionality reduction

Methods
KRR, SVM, GPR, ANN, ...

Model efficacy
Validation

Examples / challenges
Build experience and intuition

Where can I use this knowledge?

Direct

- Molecular / Materials design — Guide experiment
- Bio / Medical applications — Understand chemical process
- Method development — Widen applicability

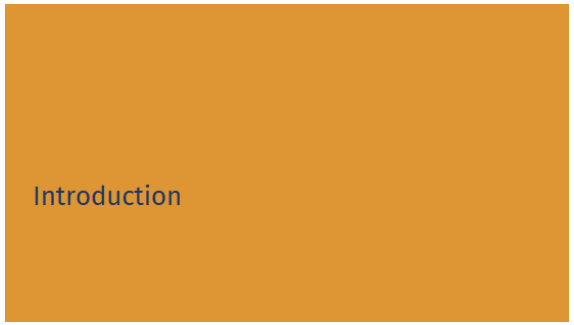
Indirect

- Data science — Extract and manage large databases
- Research in general — Strategies and methods

Lecture

Questions anytime
lecture, moodle, vonrudorff@uni-kassel.de, …
Only pre-recorded content, no live recording
Slides and notes as PDF **before** the lecture https://nablachem.org/lecture-mmc/#slides

Related: Computational Chemistry (winter term)

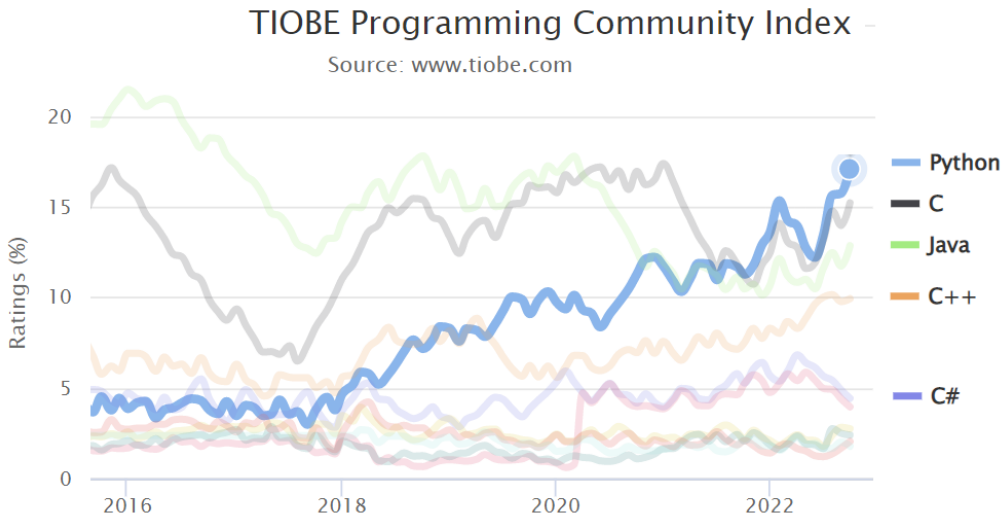


- Sections of ~30 min
- Largely self-contained
- Ask questions at latest then: new train of thought

- One slide at end of section
- Key take-aways

Exercise

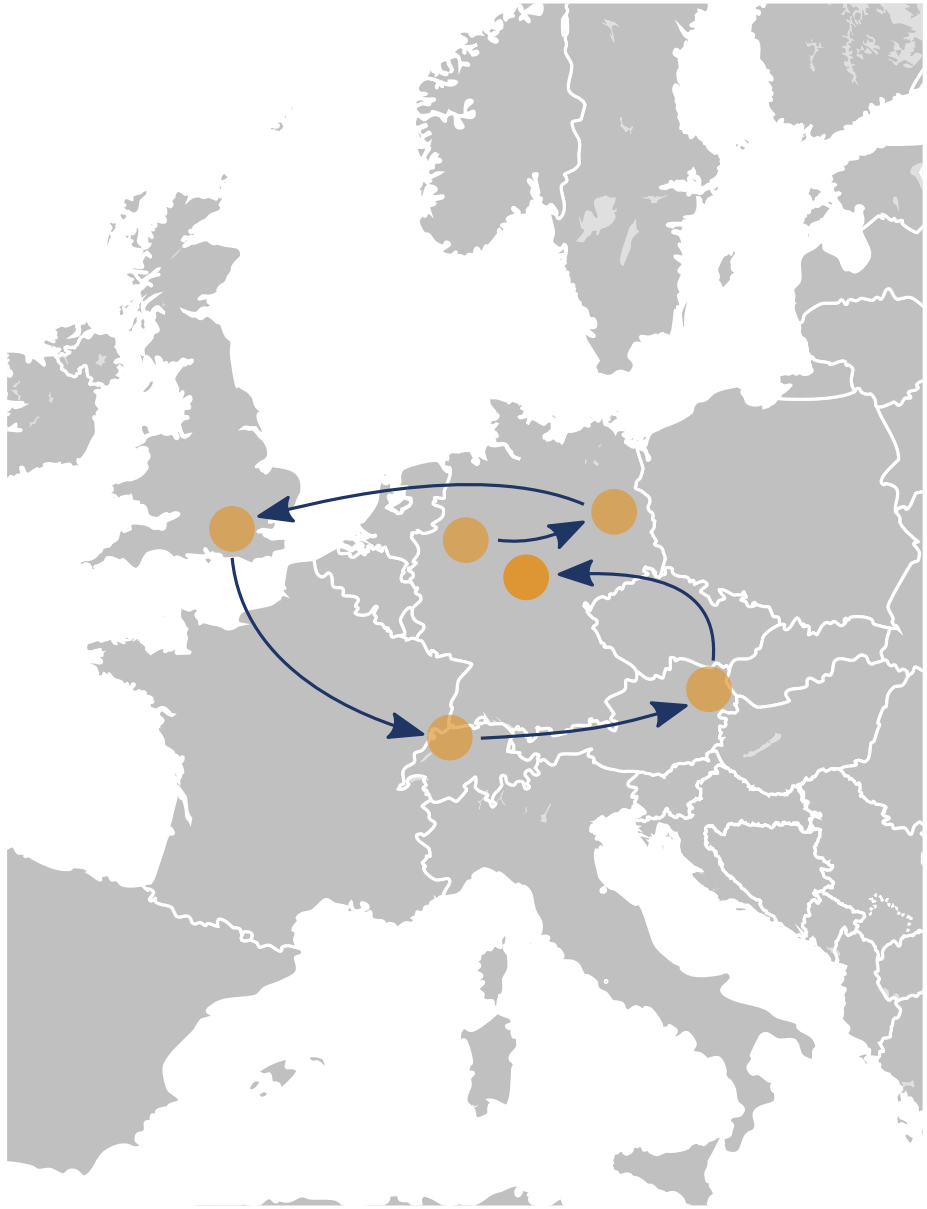
Python-based: the language of data science and glue code



Weekly assignments:

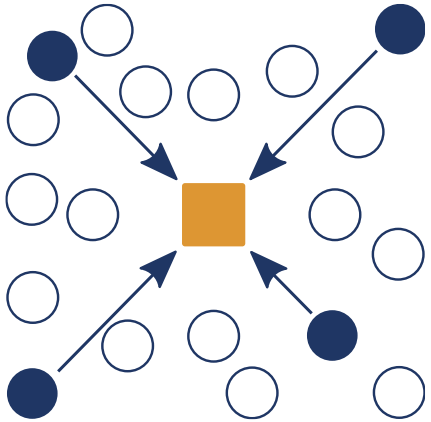
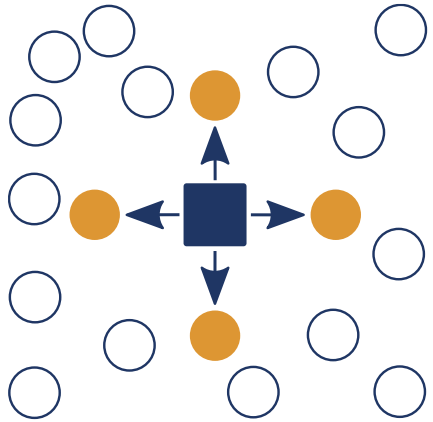
- At first: programming
- Later: machine learning
- End: modern research problems
- Typically: 2 regular tasks + one harder one if you consider research in this area

About me



BSc/MSc Physics	Berlin	Force fields
PhD Physics	London	Quantum chemistry
PostDoc	Basel, Vienna	Machine Learning & Alchemy

Machine Learning



Quantum Alchemy