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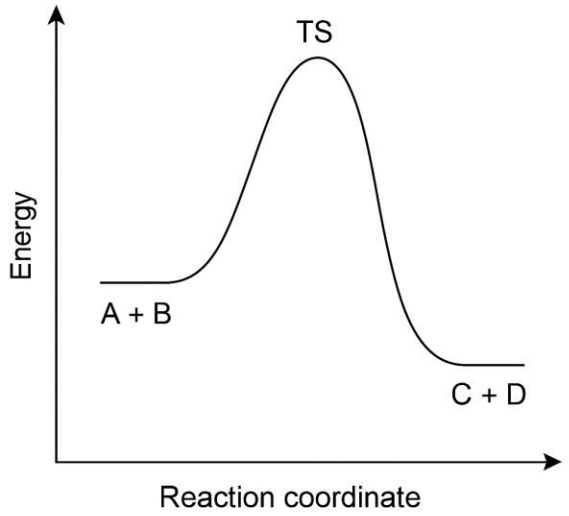
USING HPC FOR MECHANISTIC DESCRIPTION OF CHEMICAL REACTIONS

Milena Petković

УНИВЕРЗИТЕТ У БЕОГРАДУ
UNIVERSITY OF BELGRADE

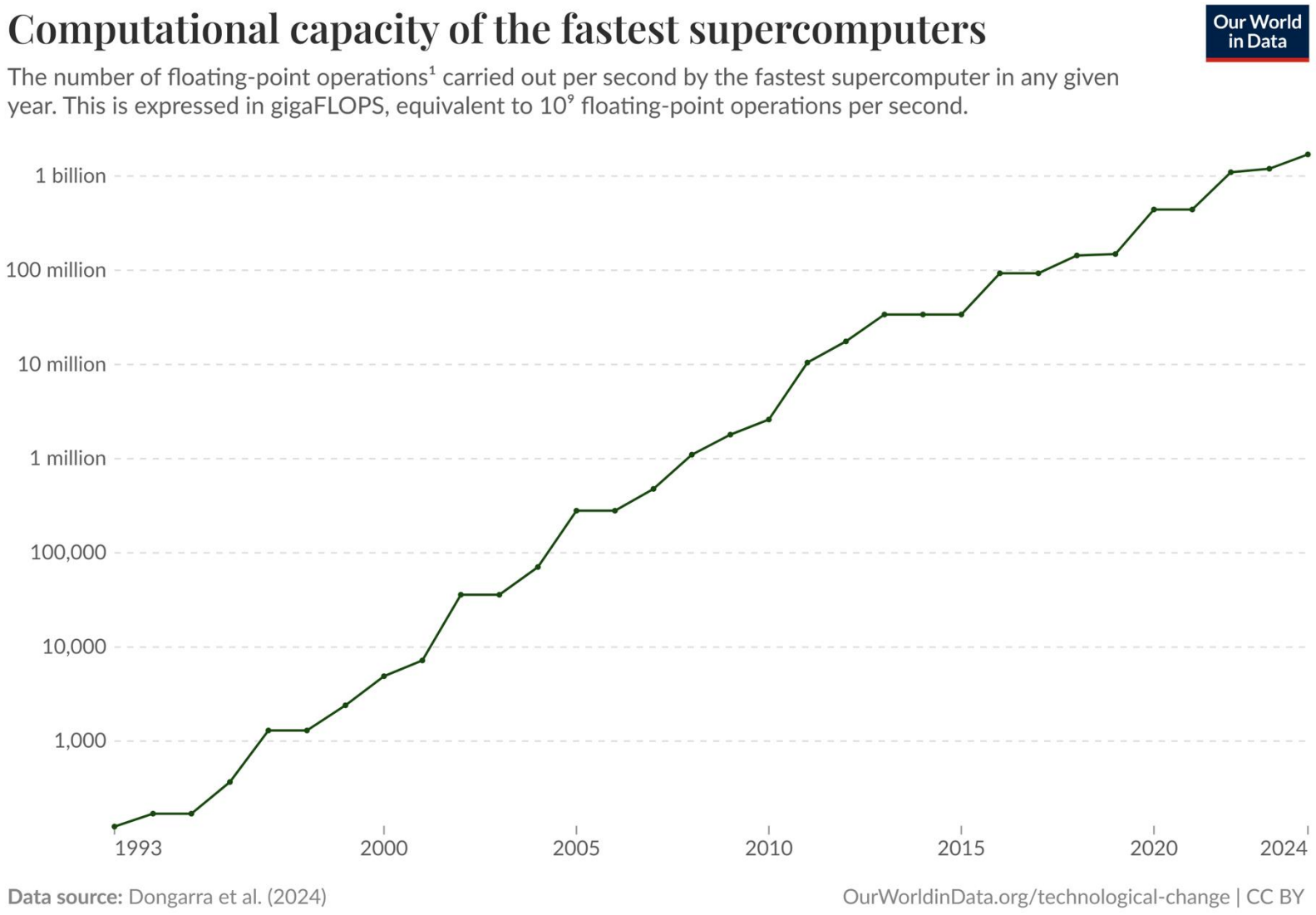
Chemical changes: importance of their detailed analysis

$A + B \rightarrow C + D$ vs.



- design of catalysts
- drug design
- manipulation of chemical reactions
- …

What a difference 30 years make



1. Floating-point operation: A floating-point operation (FLOP) is a type of computer operation. One FLOP represents a single arithmetic operation involving floating-point numbers, such as addition, subtraction, multiplication, or division.

HPC in computational chemistry

Supercomputers and parallel processing required for:

- high-level simulations
- treating large and complex systems
- performing long simulations
- sampling configurations

Types of simulations

- quantum mechanics (ab initio, DFT, semi-empirical)
- molecular mechanics
- hybrid methods (QM/MM, AIMD)
- Monte Carlo simulations

Quantum computing software

- ADF
- CP2K
- GAMESS
- Gaussian
- Molcas
- Molpro
- NWChem
- ORCA
- Q-Chem
- Quantum ESPRESSO
- TURBOMOLE
- VASP
- WIEN2k
- …

Challenges

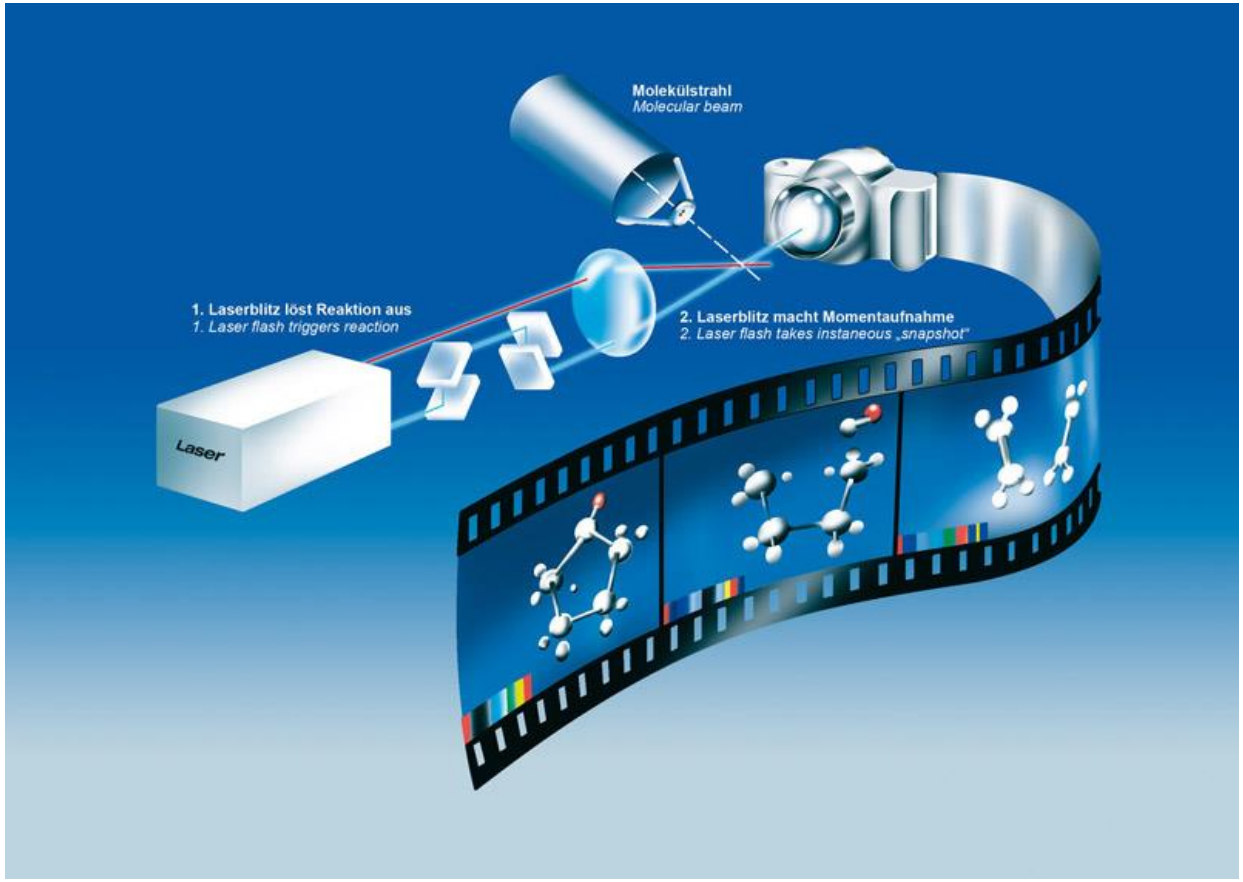
Designing a reliable model & choosing a suitable level of theory.

- high accuracy requirements
- complex reaction pathways
- multidimensional potential energy surfaces
- long simulation times
- large systems

Compromise between accuracy and computational cost.

Goal

This figure was created by experimentalists. Supercomputers enable theoreticians to design high-dimensional models that enable such a detailed descriptions of molecular transformations in the course of a chemical reaction.

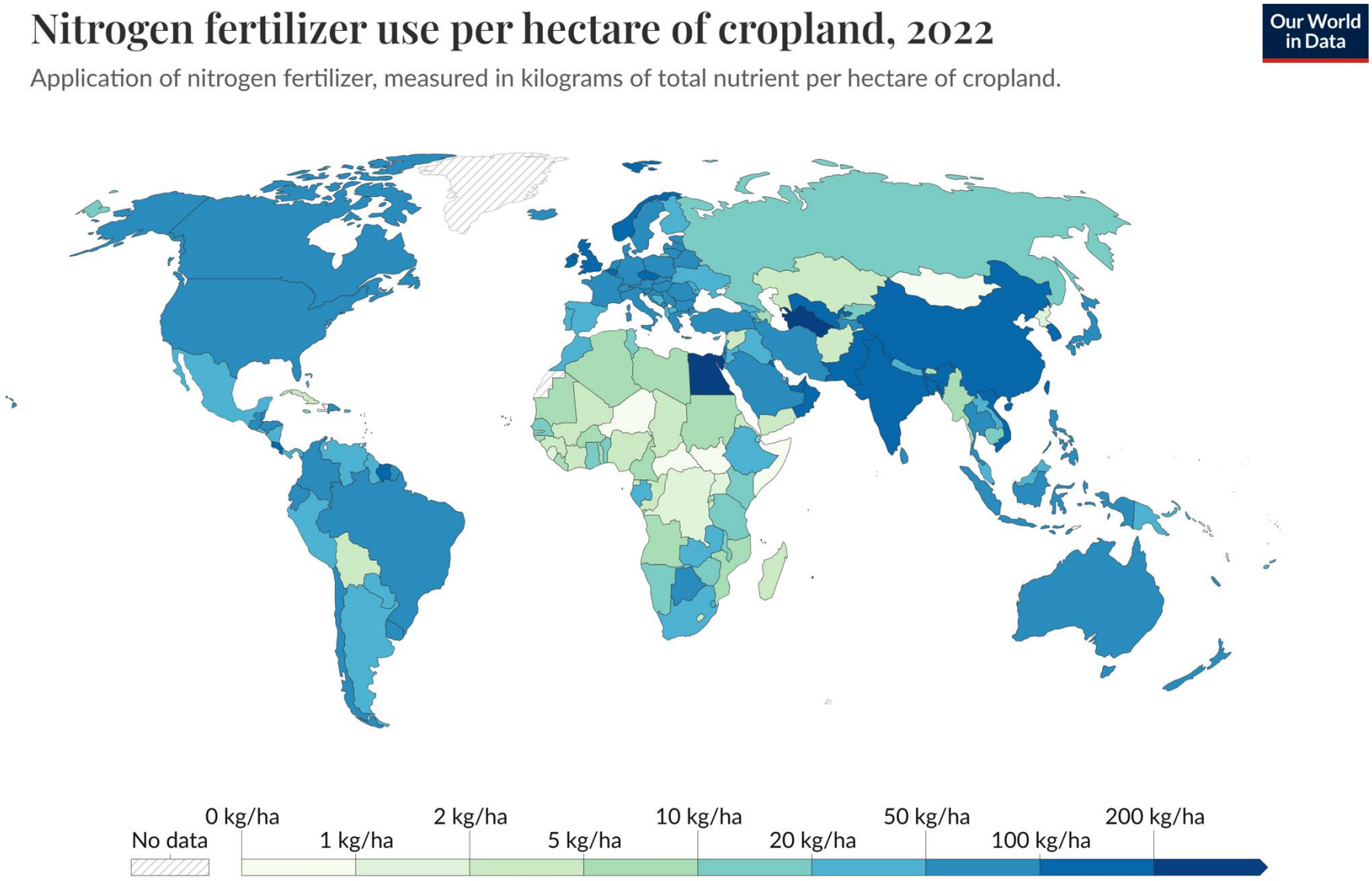


https://www.eiroforum.org/media/photo-galleries/european-xfel/attachment/femtochemie-femtochemistry/

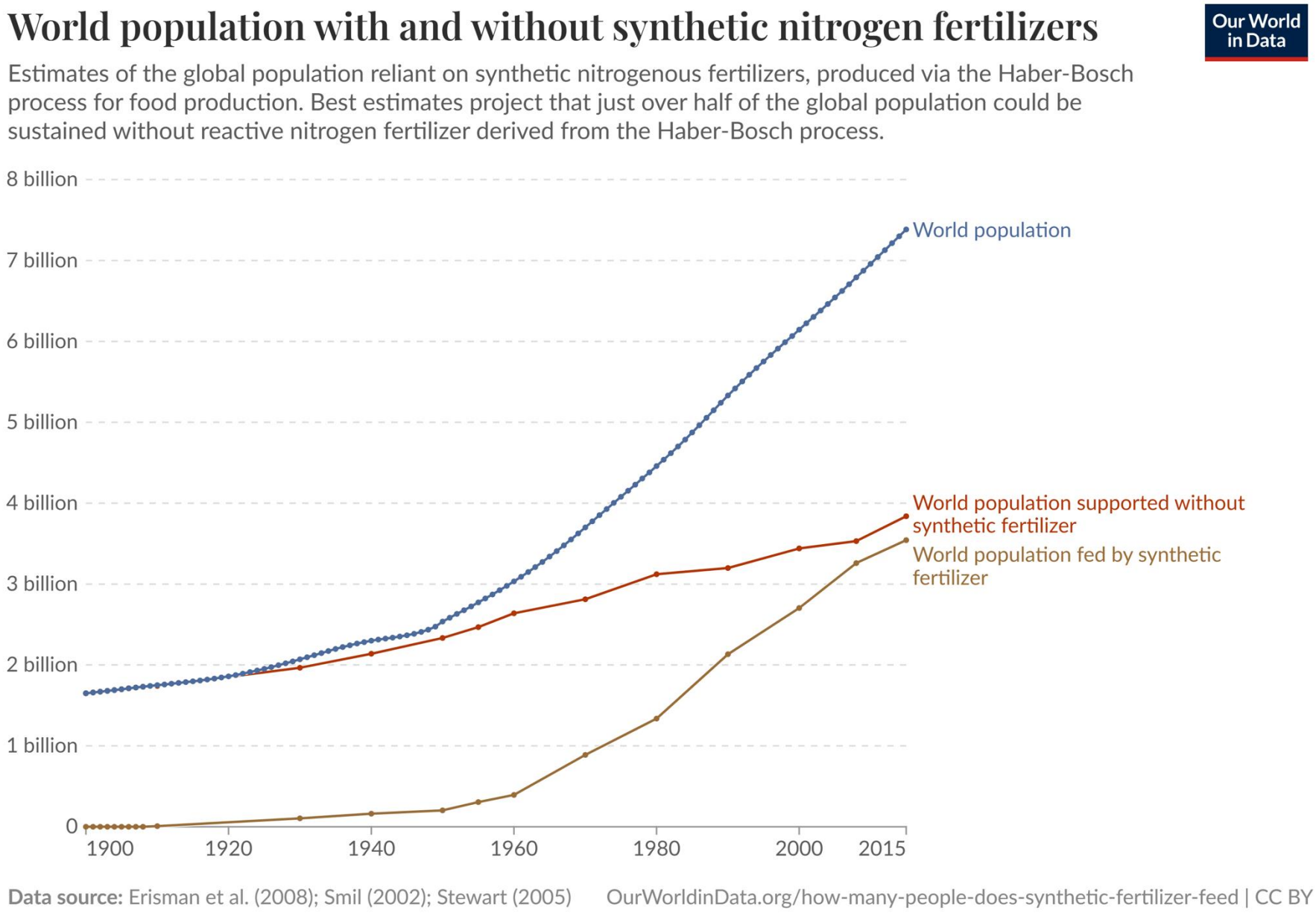
Examples

- designing catalysts
- synthetic routes that include unstable species
- reactions in the interstellar space
- light-driven reactions
- …

Case study: designing catalysts (1)



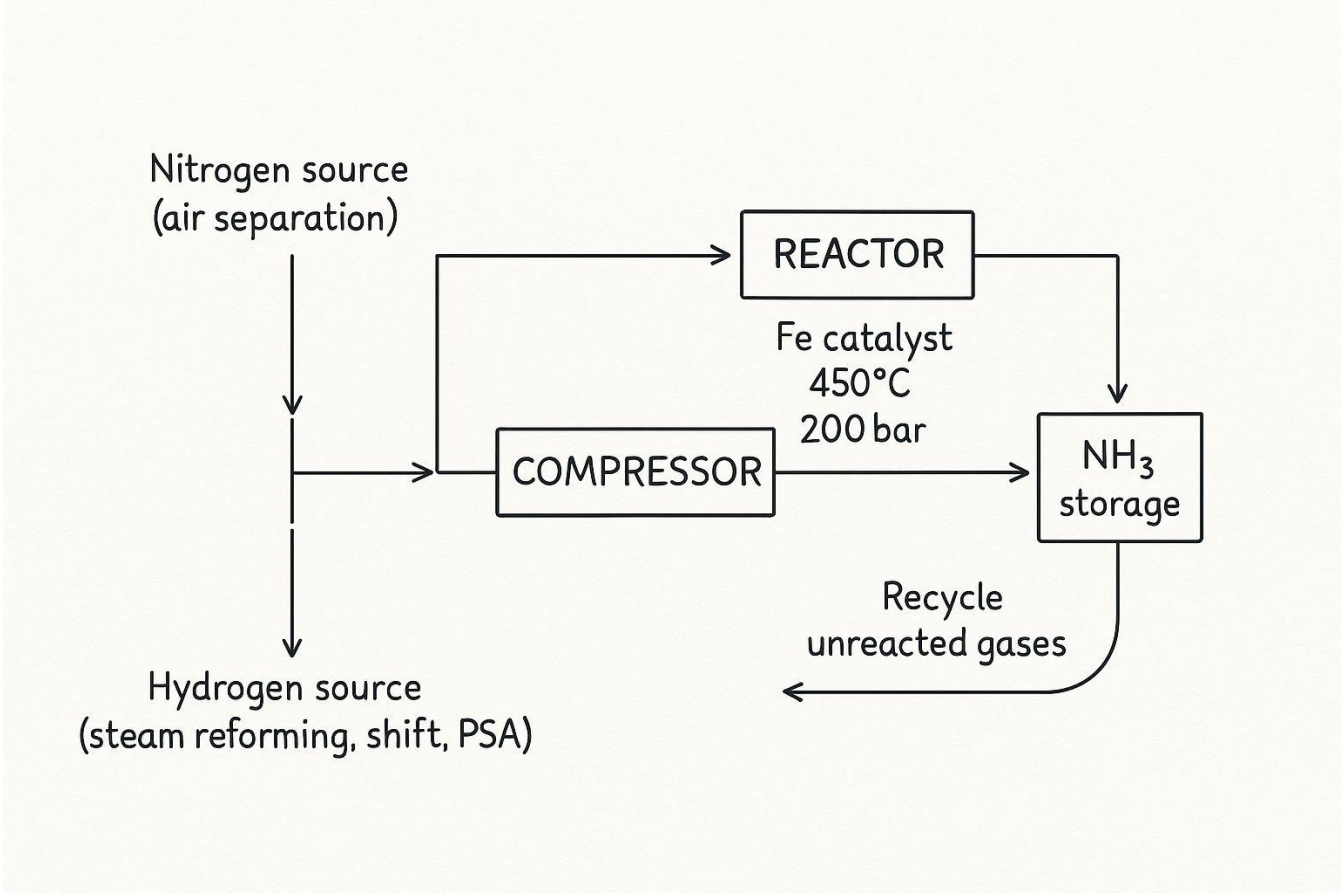
Case study: designing catalysts (2)



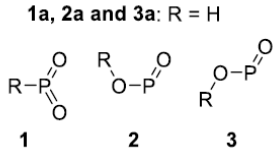
Case study: designing catalysts (3)

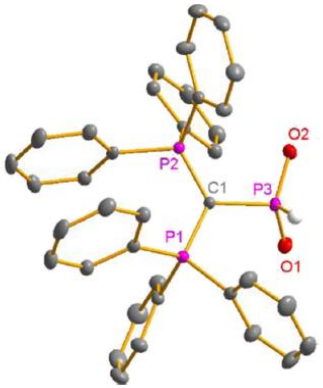
$$H_2 + 3N_2 \rightarrow 2NH_3$$

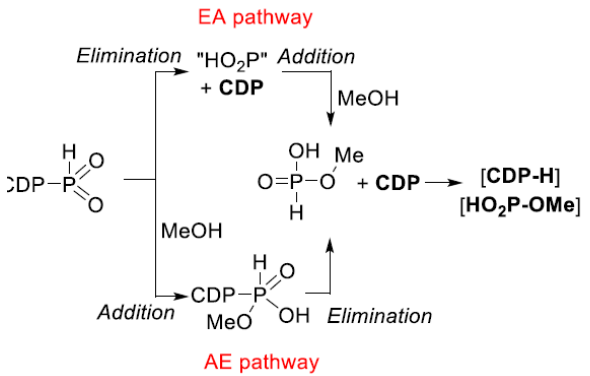
Fe catalyst → Haber-Bosch process

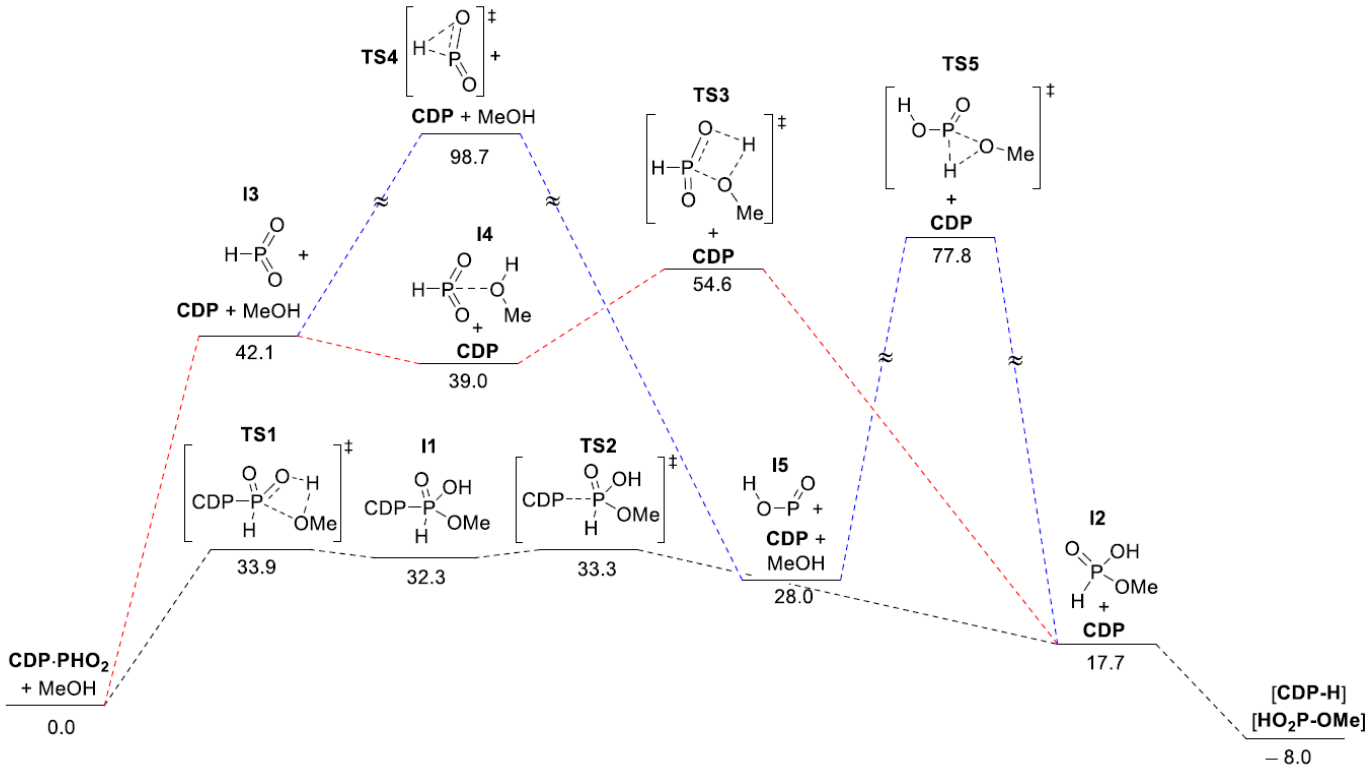


Case study: synthetic routes that include unstable species



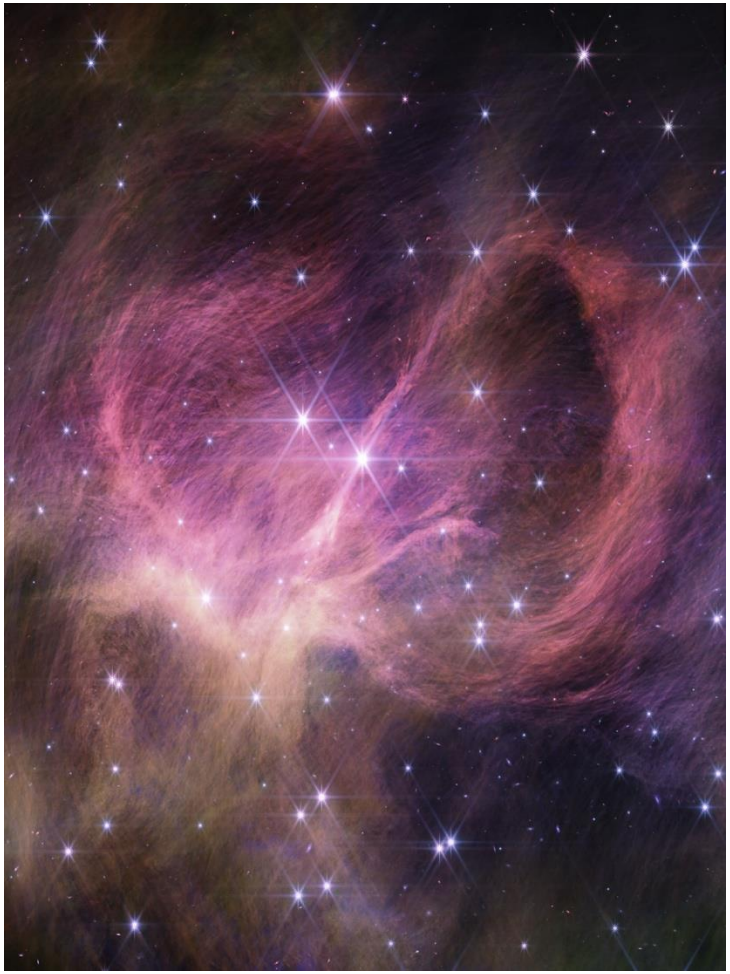






Z. Liu, A. I. McKay, L. Zhao, C. M. Forsyth, V. Jevtović, M. Petković, G. Frenking, D. Vidović, *J. Am. Chem. Soc.* 144 (2022) 7357

Case study: reactions in the interstellar space



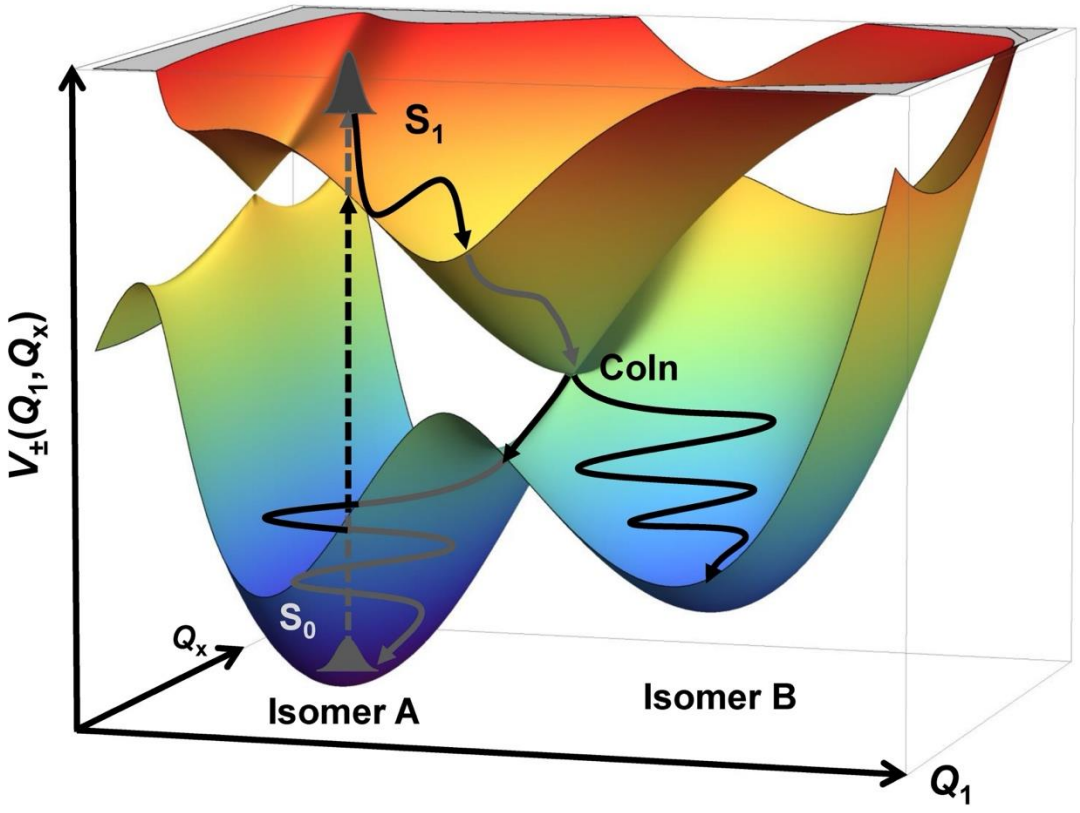
free-floating brown dwarf

- interpretation of astronomical observations
- chemical origin of stars
- formation of complex molecules

https://svs.gsfc.nasa.gov/31291/

Case study: light-driven reactions

designing high-dimensional models



https://www.temps.phc.uni-kiel.de/en/research/laboratories-and-instrumentation/femtosecond-spectroscopy

Conclusions

The progress of modern computational chemistry is tightly linked to advances in high-performance computing:

- high-level electronic structure calculations
- large systems
- long timescales

Thanks to

Institute of Physics, Belgrade

I would like to dedicate this talk to all the students and teachers who stood against corruption and the collapse of the educational system in Serbia during the 2024/2025 academic year.