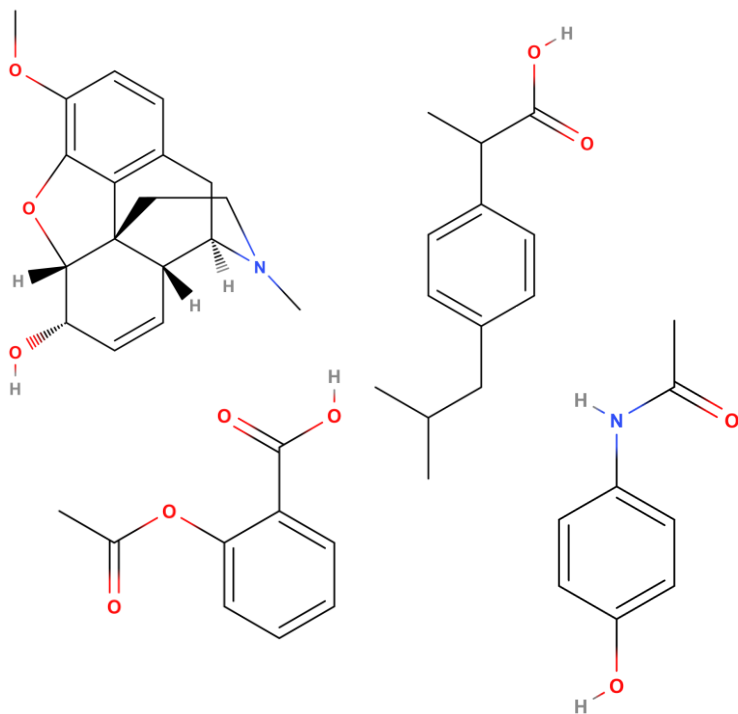


Computational Chemistry

Guido Falk von Rudorff, University of Kassel

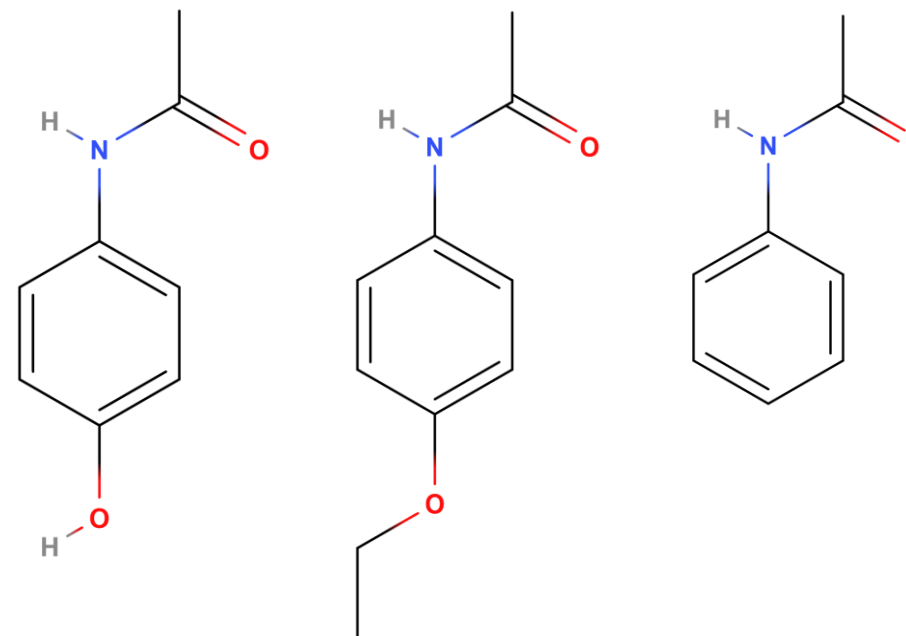


Design: sample by guided trial-and-error.



Global Search Problem

Which class of compounds?



Local Search Problem

Which particular species within that class?

Global Search Problem

Drug-like: 10^{60}

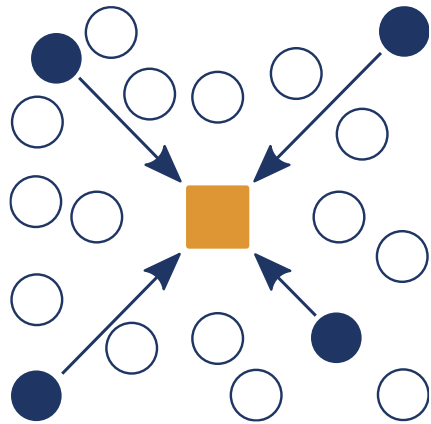
Local Search Problem

BN-doped 8x8 graphene: 10^{50}

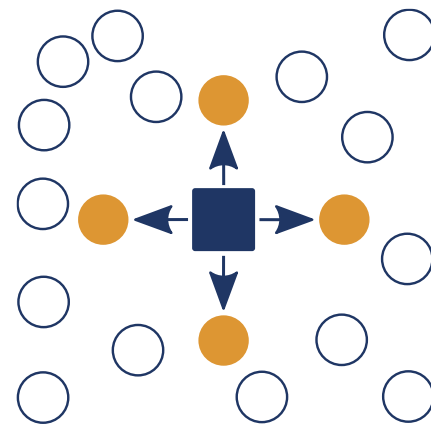
Scale

- One person: 1 million compounds/second
- 10 billion people on earth
- 10^{26} universe ages to go through

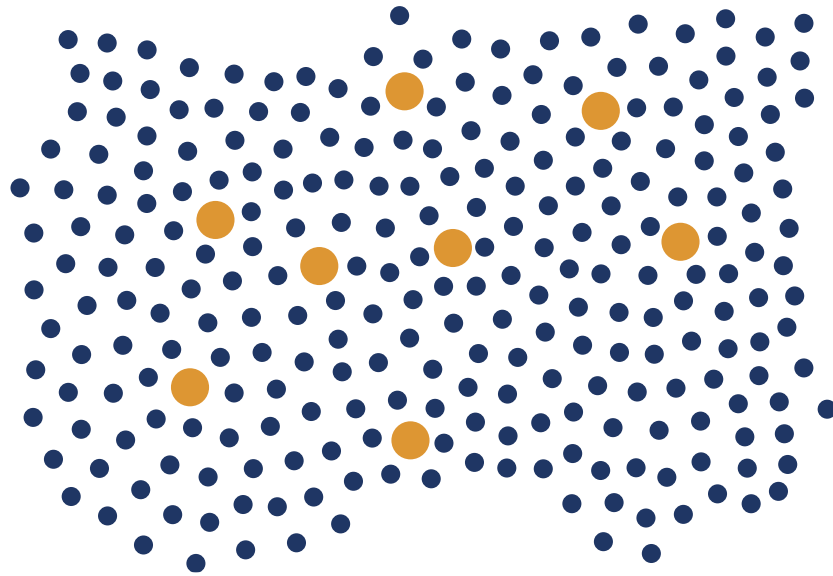
Machine Learning



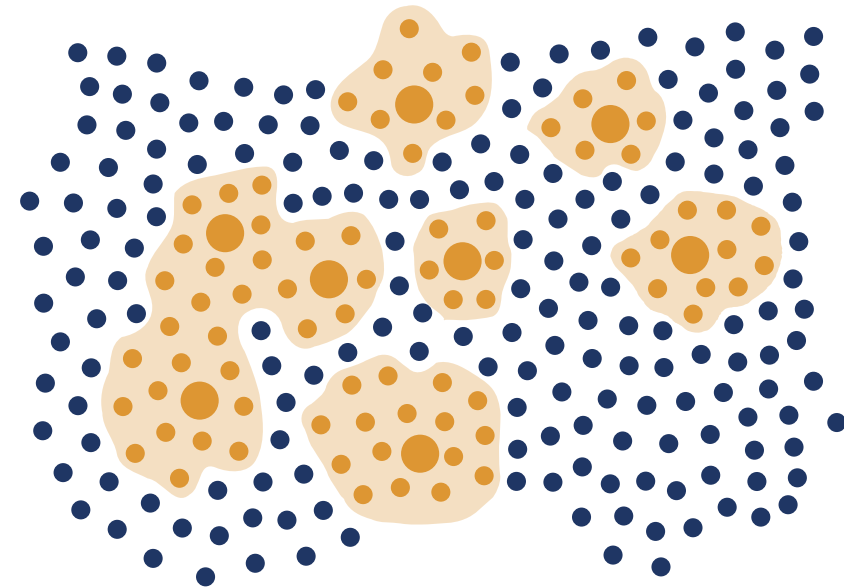
Quantum Alchemy



Without Perturbation

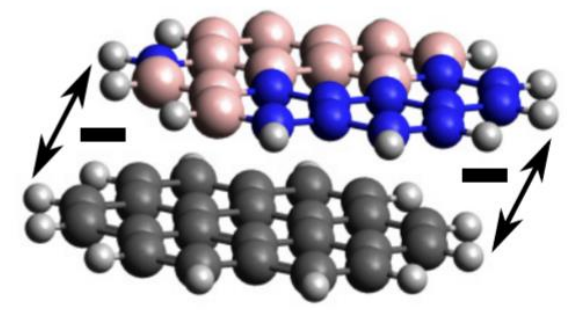
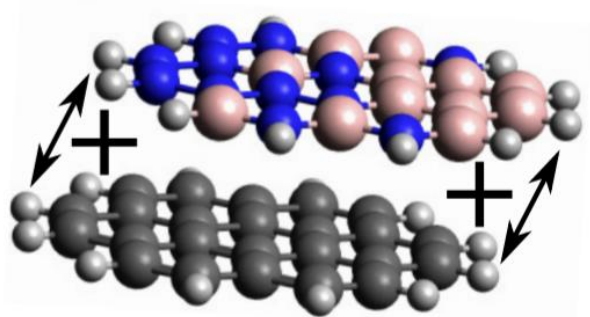
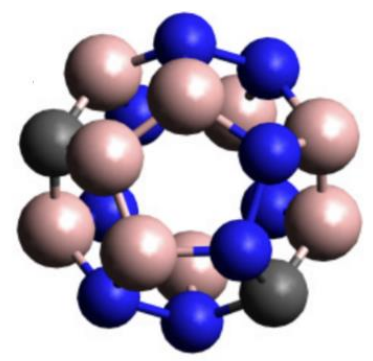
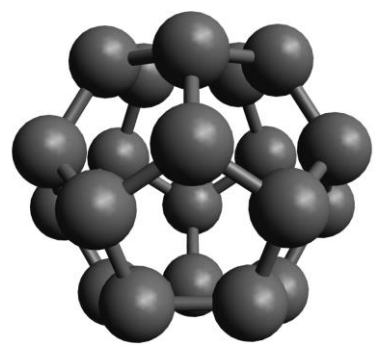
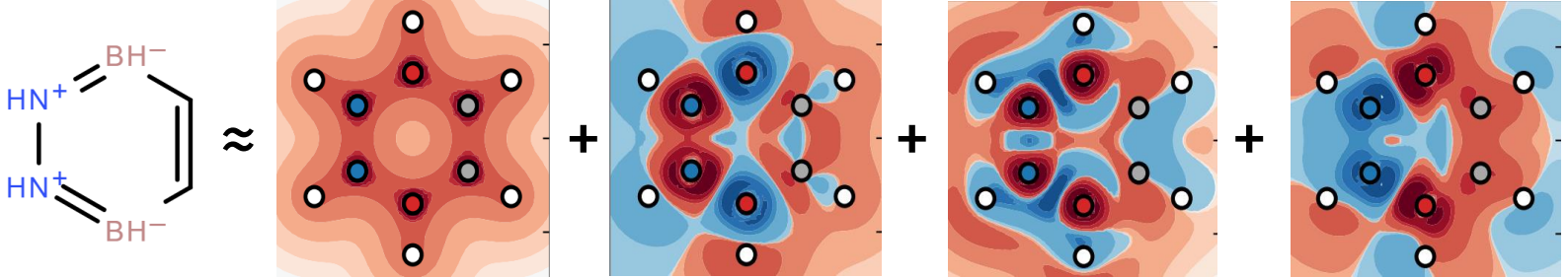


With Perturbation

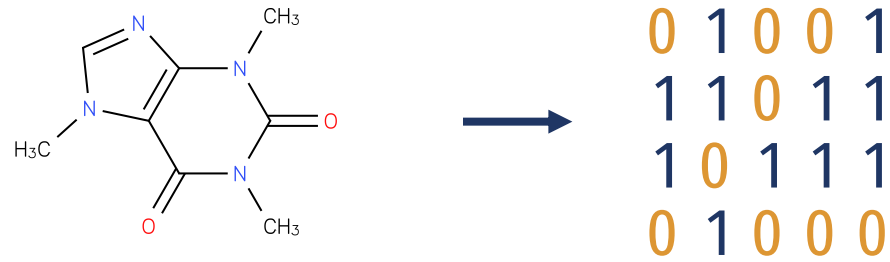


Systems/Molecules

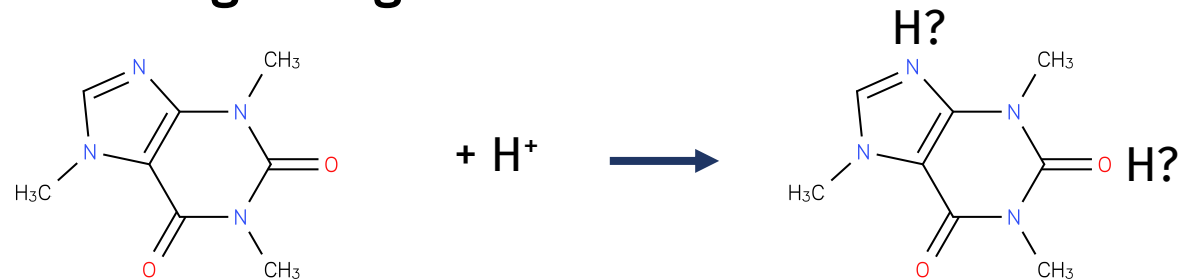
- Any
- Known
- Approximated



Kurze Moleküldarstellungen für Maschinelles Lernen



Protonierungsenergien



Molekulare Geometrien

