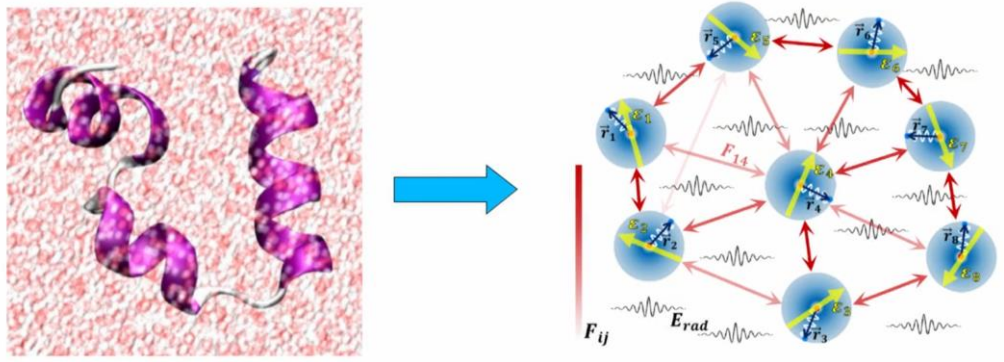
Advancing Quantum Mechanics with Mathematics and Statistics

Previously on
Advancing Quantum Mechanics with Mathematics and Statistics

Field Theory Approaches

Quantum formalism for long-range effects from atomic to large systems.



Directions:

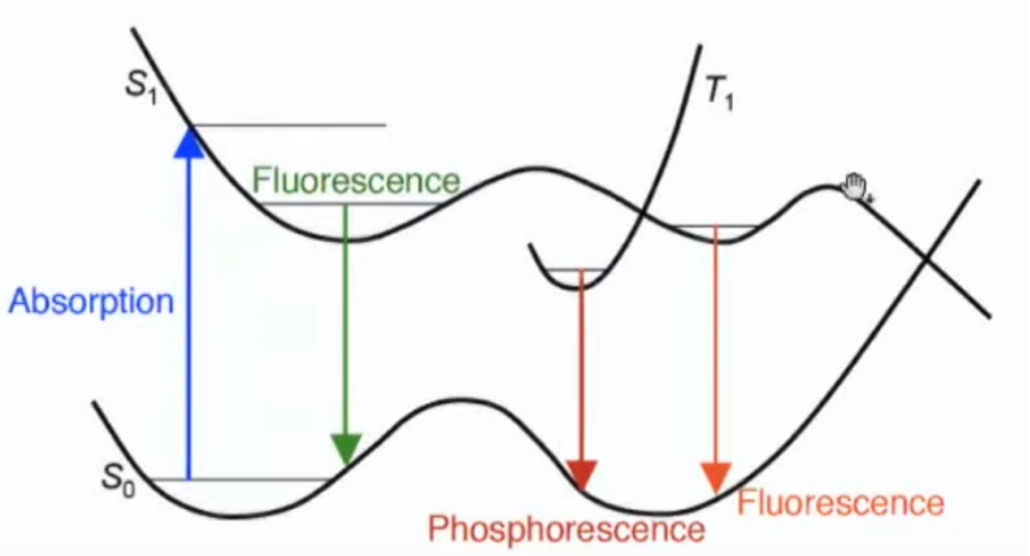
- Formal connection to (LDA-)DFT may yield new ideas on controlled approximations for XC.
- Methods for light-matter interaction

Excited and Open Quantum Systems

Propagation of excited systems or those interacting with a reservoir.

Directions:

- Accurate reference data
- Classical molecular dynamics on excited systems
- Integration with machine learning

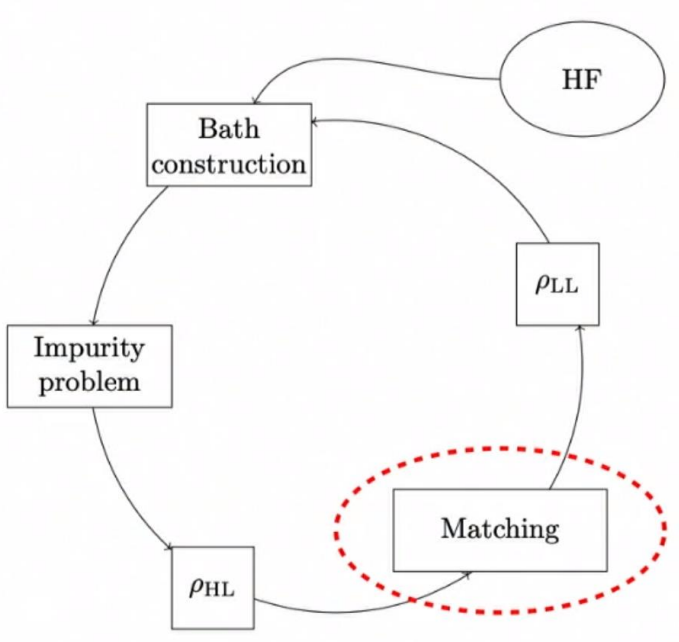


Embedding

Treat systems (e.g. defects in solids or molecules on surface) with different quantum levels or partition the problem.

Directions:

- Chemical potential fitting to constrain total number of electrons
- Bath orbital construction: general or problem-specific?
- Fragmentation strategies

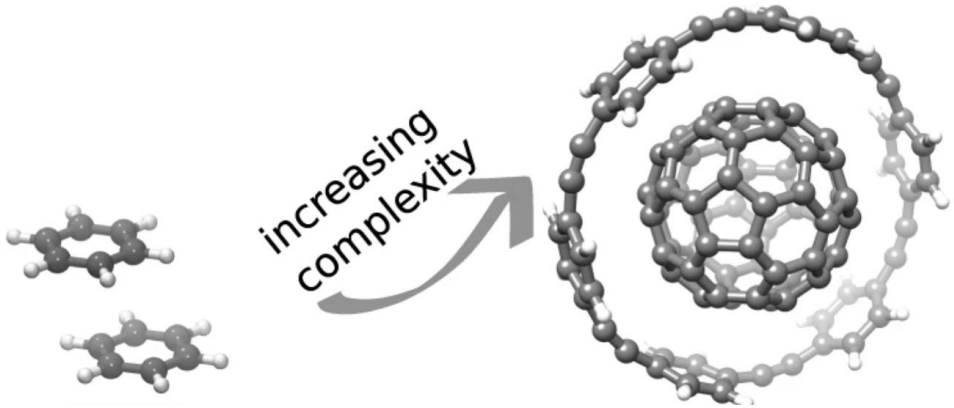


Response Functions in Molcules and Solids

Change of electronic structure w.r.t. an external perturbation.

Directions:

- Non-local response functions such as polarizability
- How to make quantum chemistry methods systematically improvable?
- Methods to obtain response functions e.g. from Quantum Monte Carlo

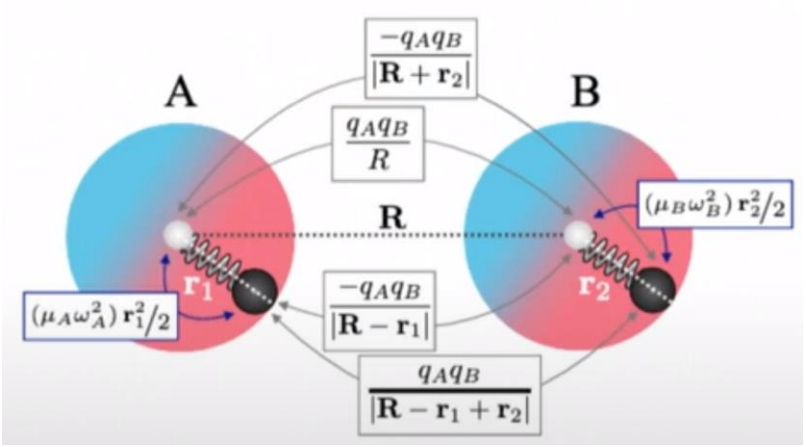


Non-covalent Interactions

Dispersion interactions from dipole fluctuations; inherently many-body and long-range.

Directions:

- Overcoming locality vs efficiency
- Combinations with machine learning without global state
- Structuring zoo of approximations



Machine Learning for Quantum Mechanics

Surrogate models enabling new domains of time and length scales.

Directions:

- Transferability with and without physical constraints
- Learning electron density for general use case
- Interpretability