Development and Applications of Quantum Chemical Methods

Jana Pavlíková Přecechtělová

jana.pavlikova@ceitec.muni.cz

Protein Structure and Dynamics,
Central European Institute of Technology, Masaryk University

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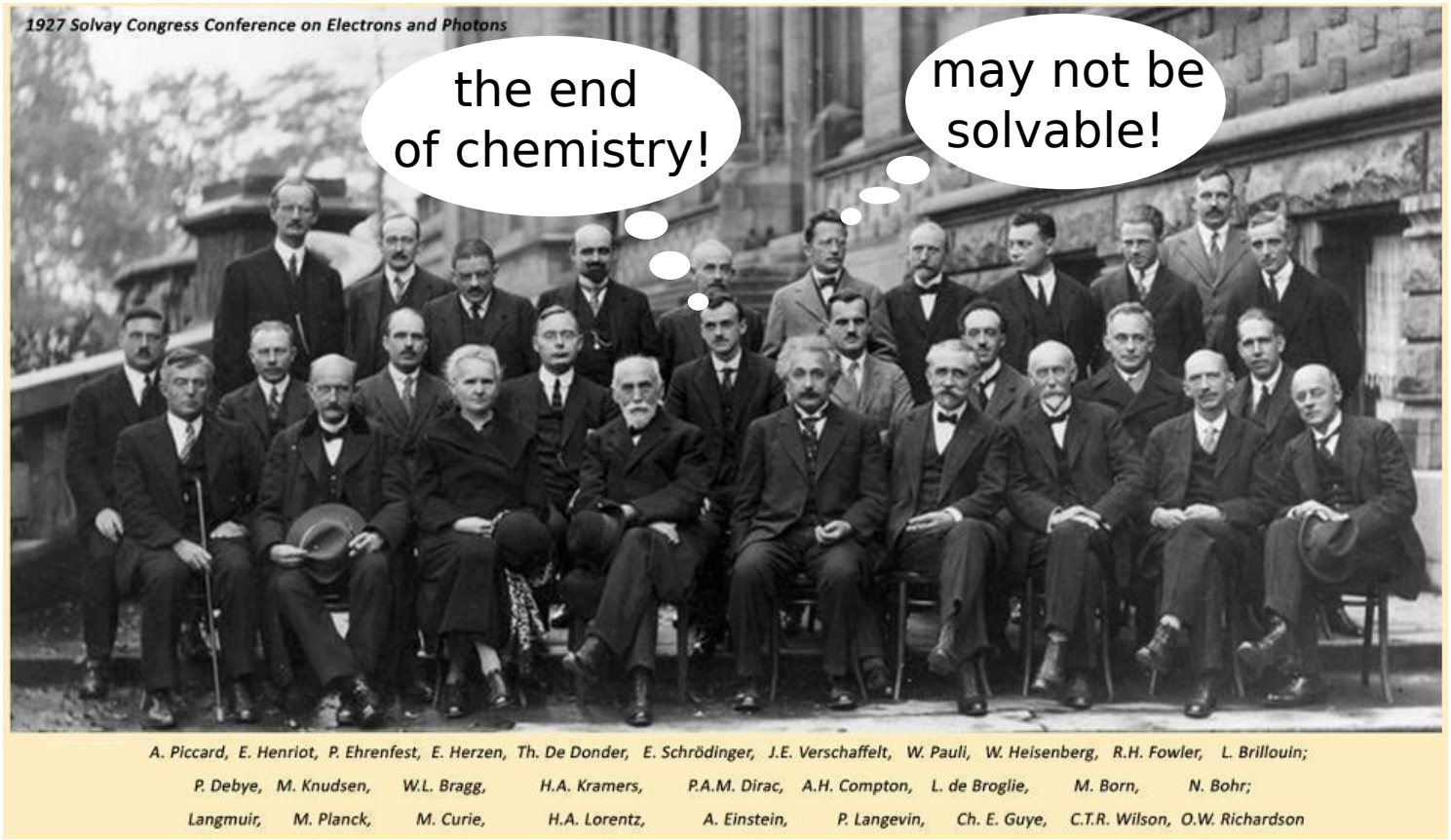
$$\hat{H}\Psi = E\Psi$$



The "wavefunction world"

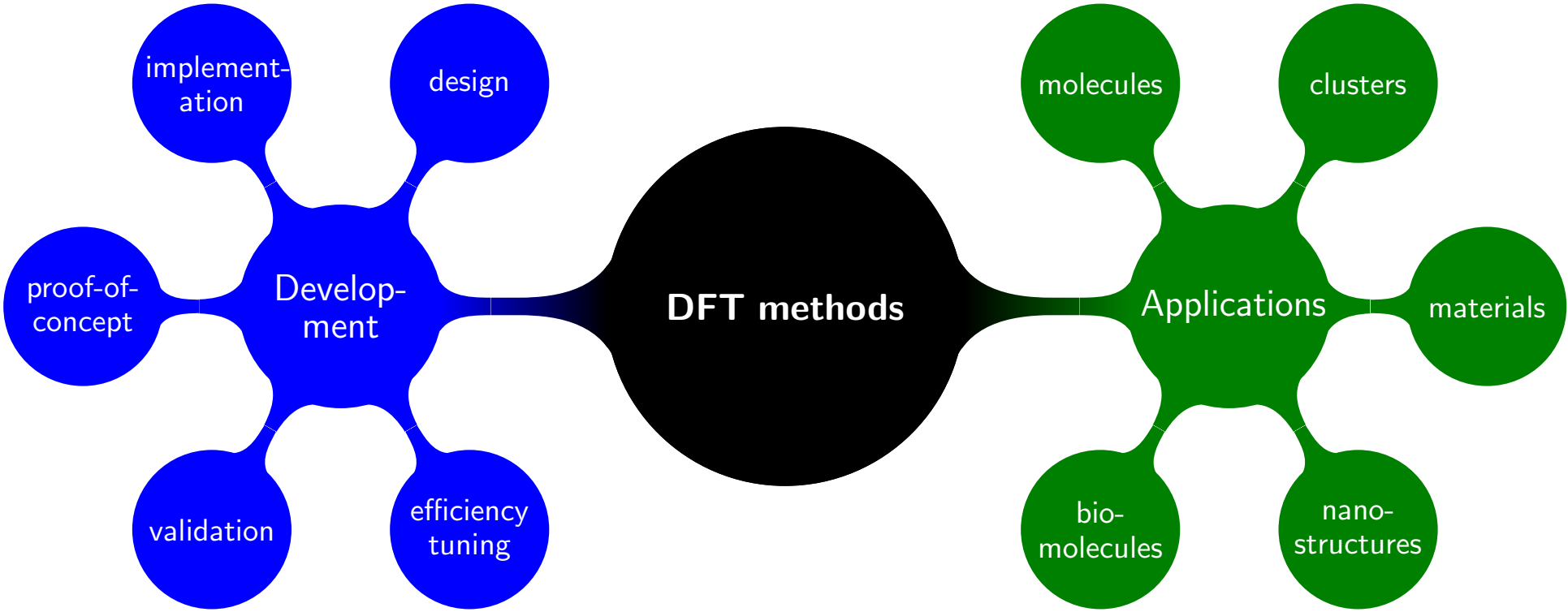
$$E_e = E_e[\Psi(\mathbf{r}_1, \mathbf{r}_2, ..., \mathbf{r}_N)]$$

$\longrightarrow$

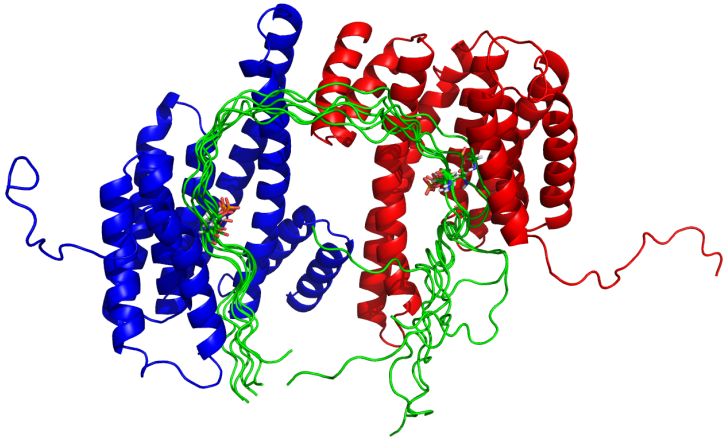
The "density world"

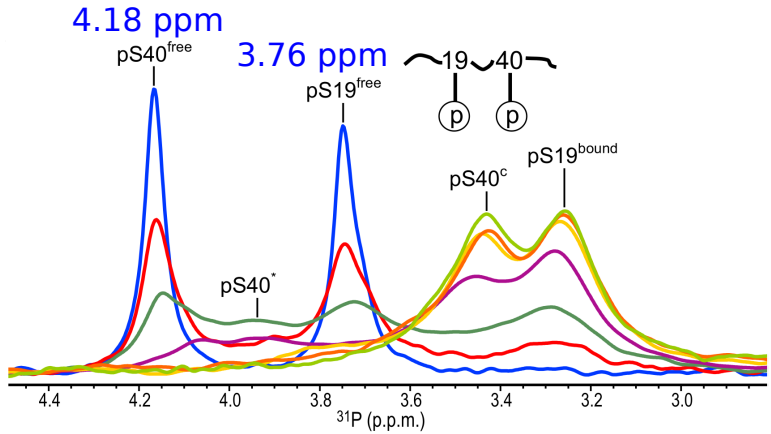
$$E_e = E_e[\rho(\mathbf{r})]$$

Research areas in density functional theory (DFT)



Project area 1: NMR calculations for proteins





Molecular dynamics → DFT calculations → statistical evaluation

↔ NMR experiment

Methods

- DFT-based fragmentation techniques
- calculations in a supercomputing environment
- scripting and programming
- molecular dynamics + NMR experiment → J. Hritz

Cooperations

- University of Tübingen
- University of Natural Resources and Life Sciences, Vienna

References

- T. Exner et al., *J. Chem. Theory Comput*, 8, 4818 (**2012**)

Project area 2: Development of density functional theory

$$E[\rho] = T_{\mathrm{s}}[\rho] + V_{\mathrm{Ne}}[\rho] + J[\rho] + E_{\mathrm{XC}}[\rho]$$

$E[\rho]$: el. energy

$T_{\mathrm{s}}[\rho]$: kinetic energy

$V_{\mathrm{Ne}}[\rho]$: nuclear electron attraction

$J[\rho]$: Coulomb repulsion

$E_{\mathrm{XC}}[\rho]$: exchange-correlation energy functional — unknown!!!

must be approximated!!!

Exchange-correlation functional

$$E_{\mathrm{XC}} = \int \mathrm{d}\mathbf{r}\ \rho \int \mathrm{d}u\ 2\pi u\, \rho_{\mathrm{XC}}$$

Correlation factor approach

$$\rho_{\mathrm{XC}}(\mathbf{r}, u) = \rho_{\mathrm{X}}(\mathbf{r}, u) f_{\mathrm{C}}(\mathbf{r}, u)$$

Methods

- Design of new mathematical models for ρ_{XC}, f_{C}

  Mathematica
- Implementation into commercial software codes

  Gaussian, Fortran
- Validation of correlation-factor-based functionals

  atomization energies, barrier heights . . .

Cooperations

- University of Montreal
- Technical University Berlin

References

- Bc. thesis of Tomáš Persaň
- J. Pavlíková Přecechtělová, *J. Chem. Phys.*, **2015**

Contact

jana.pavlikova@ceitec.muni.cz

building A14

room 2.16 or 2.25