Time-Dependent Density Functional Methods for Description of Excited States Properties

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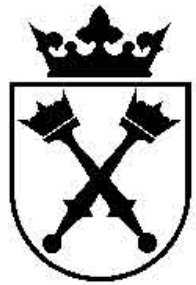

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Problem

- What?
  - to benchmark TD-DFT methods against very accurate experimental data
- Why?
  - to make the choice of exchange-correlation functional more science than art
- How?
  - systems: atoms and small molecules
  - experiment: accurate adiabatic excitation energies, bondlengths and frequencies
  - computations: rich choice of functionals, TDA and RPA variants of TD-DFT, large basis sets, quality grids

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- hybrid (screened-hybrid) functionals more accurate than pure ones
- CAM-B3LYP in TDA variant is the most robust
- when CAM-B3LYP fails simple local SVWN functional gives decent energetics, but:
  - physical explanation of this effect is unclear
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