Computational Materials Physics

Center for Molecular Modeling

Department of Materials Science and Engineering

Hartree-Fock vs. DFT

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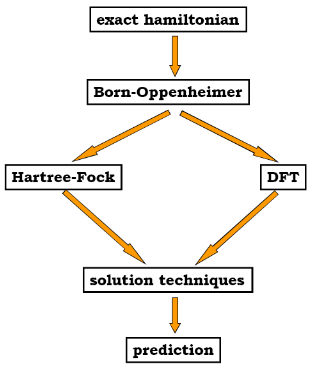
http://molmod.ugent.be
http://www.ugent.be/ea/dmse/en
my talks on Youtube: http://goo.gl/P2b1Hs

three levels of approximations

level 1:

level 2:

level 3:



HF vs. DFT

Hartree-Fock	DFT (exact)
exact exchange (by definition) no correlation (by definition)	$E_{xc}[\rho]$ contains exact exchange and exact correlation
correlation to be included by post-HF treatments: • step by step • computationally lengthy	Solving KS-equations with this $E_{xc}[\rho]$ gives exact result

HF vs. DFT

Hartree-Fock

exact exchange (by definition)
no correlation (by definition)

correlation to be included by post-HF treatments:

- step by step
- computationally lengthy

DFT (LDA)

$E_{xc}^{LDA}[\rho]$ contains some exchange and some correlation

Solving KS-equations with $E_{xc}^{LDA}[\rho]$ gives approximate result

HF vs. DFT

Hartree-Fock

exact exchange (by definition)
no correlation (by definition)

correlation to be included by post-HF treatments:

- step by step
- computationally lengthy

DFT (LDA)

$E_{xc}^{LDA}[\rho]$ contains some exchange and some correlation

Solving KS-equations with $E_{xc}^{LDA}[\rho]$ gives approximate result

Improvements require black magic

HF vs. DFT

The same message, but now told in a more graphical way:

HF vs. DFT

first principles

Goal :

HF vs. DFT

first principles

Goal :

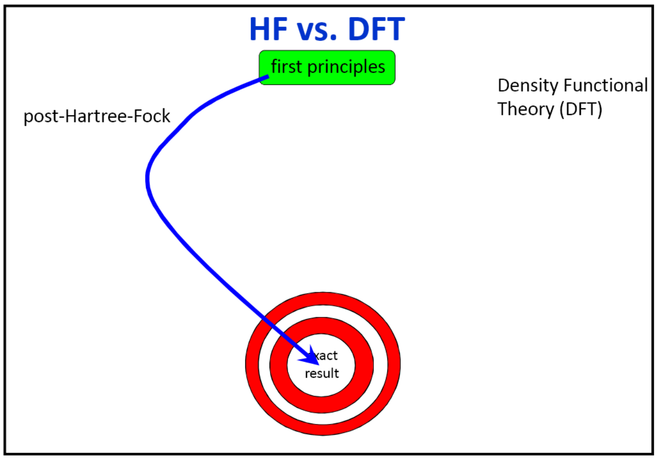
HF vs. DFT

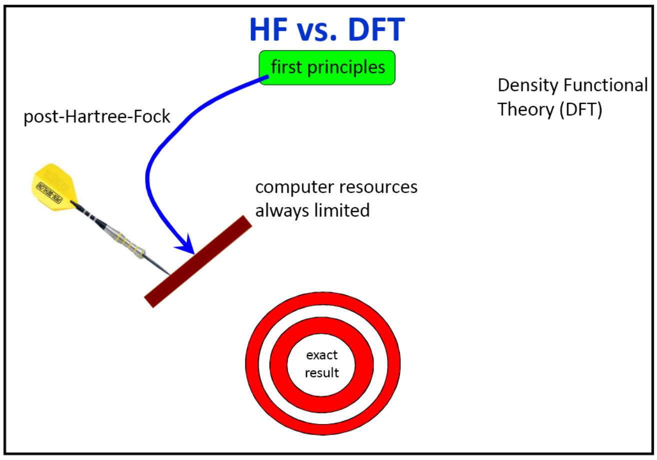
first principles

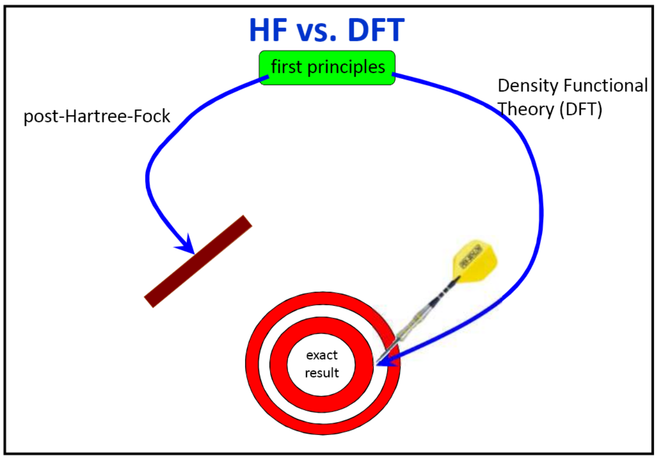
Schrödinger (or Dirac) equation

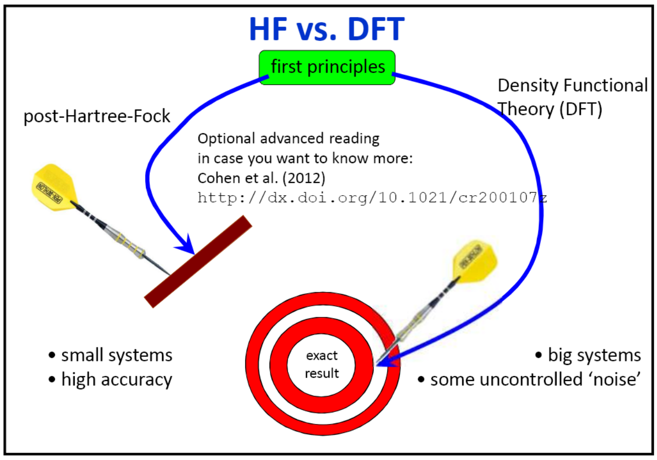
Goal :

"simply solve it"


HF vs. DFT
first principles
post-Hartree-Fock
Density Functional Theory (DFT)
result


HF vs. DFT
first principles
post-Hartree-Fock
Density Functional Theory (DFT)
computer resources always limited
exact result


HF vs. DFT
first principles
post-Hartree-Fock
Density Functional Theory (DFT)
exact result


HF vs. DFT
first principles
post-Hartree-Fock
Density Functional Theory (DFT)
Optional advanced reading
in case you want to know more:
Cohen et al. (2012)
http://dx.doi.org/10.1021/cr200107z
exact result
• small systems
• high accuracy
• big systems
• some uncontrolled 'noise'