„Repelling Electrons United in Harmony"

– „Sich abstoßende Electronen vereint in Harmonie" –

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PhD defense

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Why are we here? – Definitions

I have to earn my PhD!

give a talk

about my scientific work

only true in Germany: PhD ≙ Dr. rer. nat.

Doctor rerum naturalium ... Doctor of Science

in general (international context)

PhD ... Doctor of Philosophy

$\Longrightarrow$ I give a philosophical talk!

PhD... Doctor of Philosophy – more specific

Doctor... latin: docēre ≙ to teach

Philosophy... ancient greek: φιλοσοφια ≙ love of wisdom

earn my PhD

⇒ I have <u>to teach</u> you <u>to love</u> <u>wisdom</u>

× not schooling

o awake the will to learn

like it

deep understanding of relationships in nature

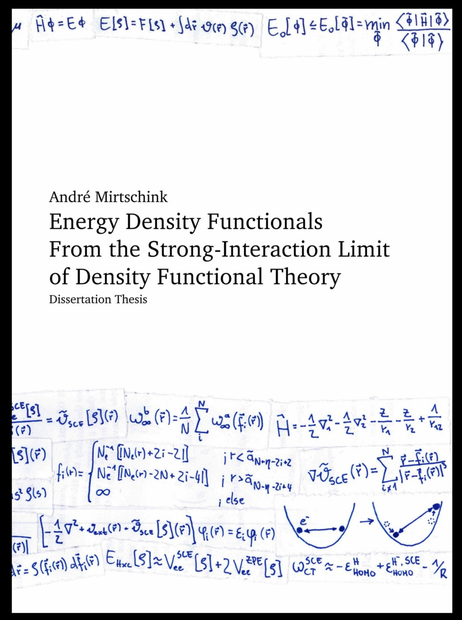
⇒ trigger your curiosity with <u>interesting</u> <u>knowledge</u>

Interesting Knowledge

my knowledge

$\hat{=}$

my thesis



is it really interesting?

a few say yes,

but most say no ...

Anyway, Let my try!

My Thesis - Interesting!

begin: „to everyone supporting me"
end: „I am a product of my environment"

no shadow without light

no good without evil

male - female

interesting thought ... why? it's harmonic

- combination of apparently opposite
- very natural principle

More Harmony in my Thesis?

Yes, the <u>KS-SCE method</u>!

predicts properties of atomic matter by <u>efficient</u> computer simulations

<u>high accuracy</u> at <u>low numerical cost</u>

seems in contrast Hohenberg-Kohn 1964 promis <u>Harmony</u>

deep understanding of electronic nature $\xrightarrow{\text{Schrödinger 1926}}$ <u>very complex</u>

- e^- are quantum mechanical objects
- e^- repel each other

$\hat{=}$ e^- like to travel and tend to fight

! still, e^- live in <u>harmony</u> (stable atoms, chemical bonds)

Schrödinger:

life experience $\hat{=}$ takes time

Hohenberg-Kohn:

education $\hat{=}$ <u>very efficient</u>

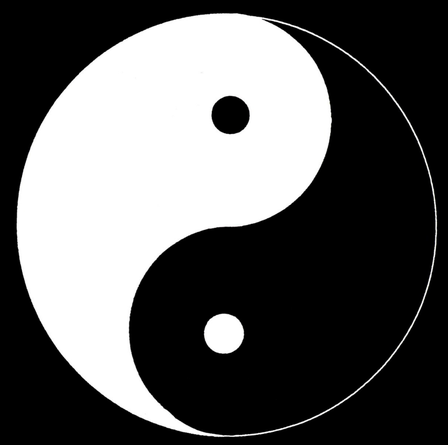
KS-SCE School of Harmony

- est. 1964 by Hohenberg and Kohn
- lectures on density functional theory

DFT I – KS
Kohn-Sham 1965

- e^- don't repel each other
- e^- are QM particles
  $\hat{=}$ charge clouds

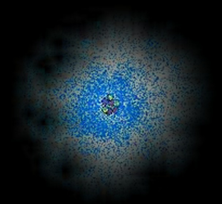
$\Rightarrow$ e^- learn to travel, but are very naive



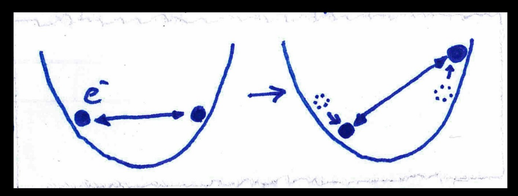
DFT II – SCE
Seidl–Gori-Giorgi –Savin 2007

- e^- repulsion is infinitely strong
- ∞ e^- are classical particles
  $\hat{=}$ point charges

$\Rightarrow$ e^- avoid each other



$\Rightarrow$ e^- live in harmony!



↯ Though they avoid each other too much ... e^- with anxiety disorder ↙

$\Rightarrow$ course DFT III to come:

„Psychotherapy for e^-"

„to everyone supporting me"

I hope you did like my wisdom!?

Thanks a lot!