



Center for Molecular Modeling

# Computational Materials Physics



Department of Materials Science and Engineering

## DFT teaser

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

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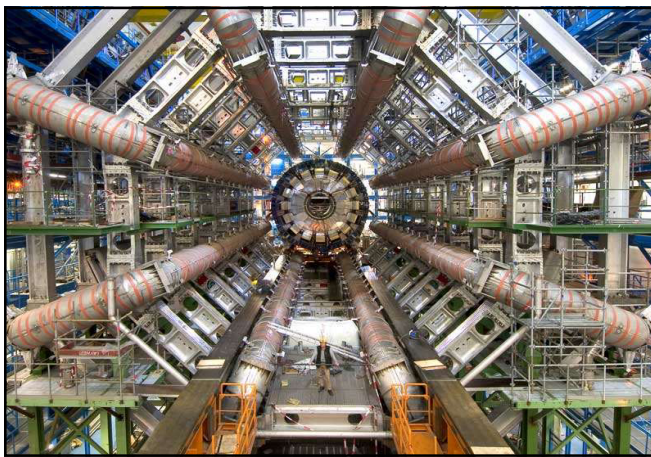
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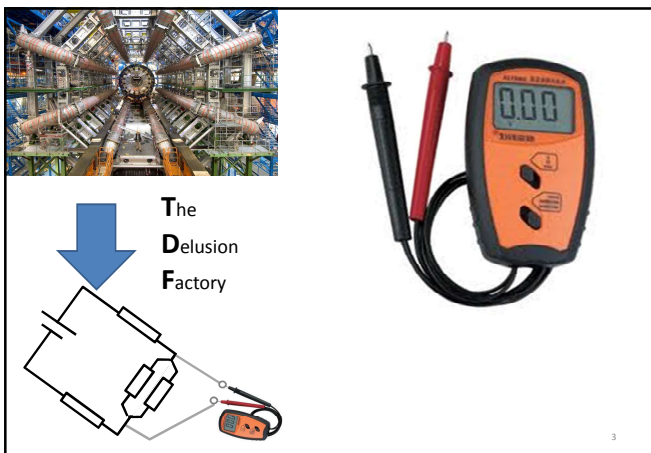
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**The Delusion Factory**

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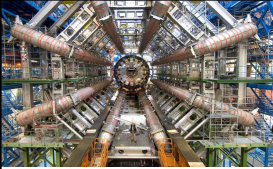
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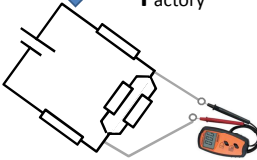
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**The Delusion Factory**

↓



$$\hat{H} \Psi(\vec{r}_1, \dots, \vec{r}_N) = E \Psi(\vec{r}_1, \dots, \vec{r}_N)$$

many-body Schrödinger equation

**Density Functional Theory** ↓

$$\hat{H}_{KS} \phi(\vec{r}) = E \phi(\vec{r})$$

single-particle Kohn-Sham equations

methods: LAPW, PAW, grids, ...  
codes: VASP, QE, WIEN2k, ...

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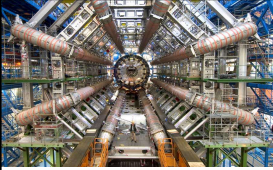
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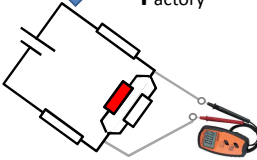
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↓



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many-body Schrödinger equation

**Density Functional Theory** ↓ **XC?**

$$\hat{H}_{KS} \phi(\vec{r}) = E \phi(\vec{r})$$

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