Calculation of nmr parameters in paramagnetic metal-organic materials

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Presentation plan

1. MOFs = Metal—organic frameworks

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2. NMR — what and why

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5. Preliminary results

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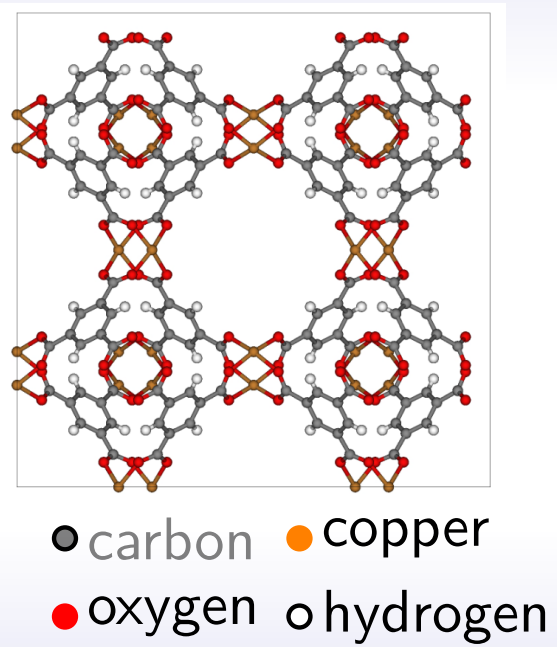

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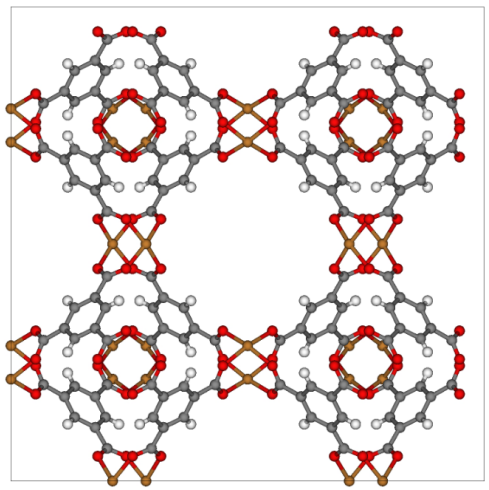

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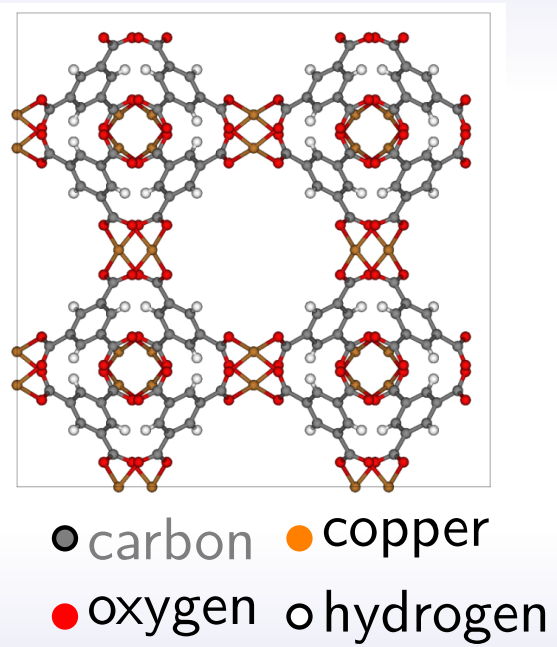

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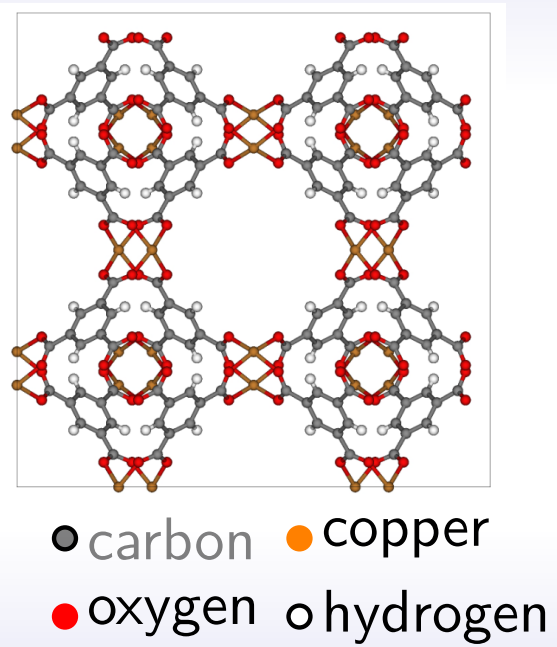

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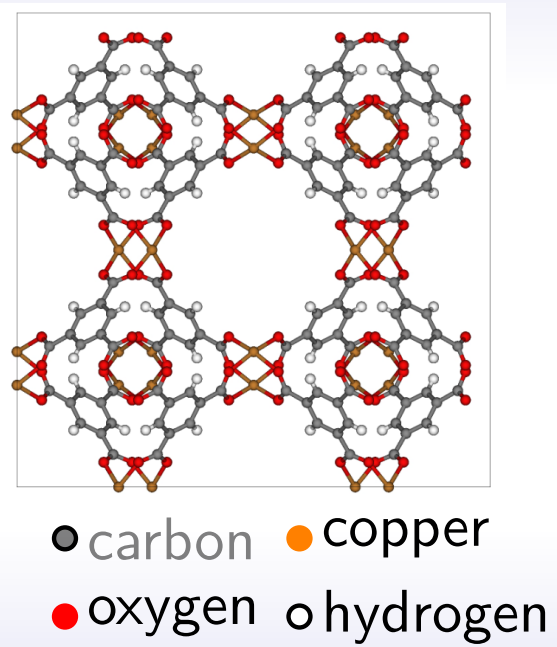
- NMR spectra feature large shifts caused by unpaired electrons



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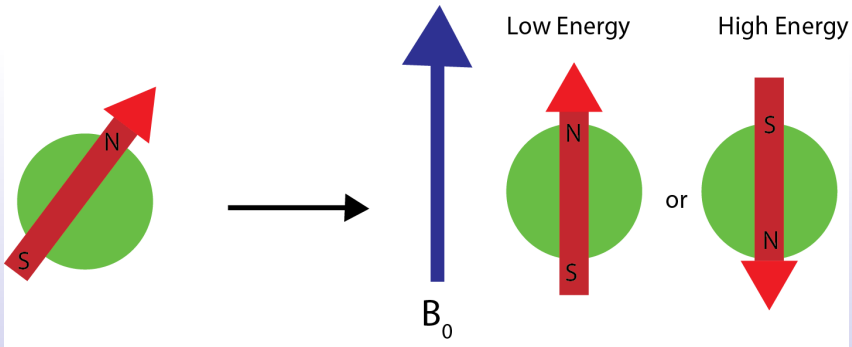

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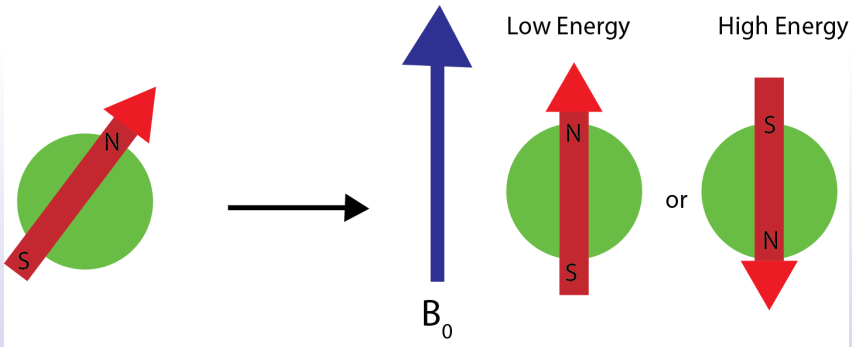

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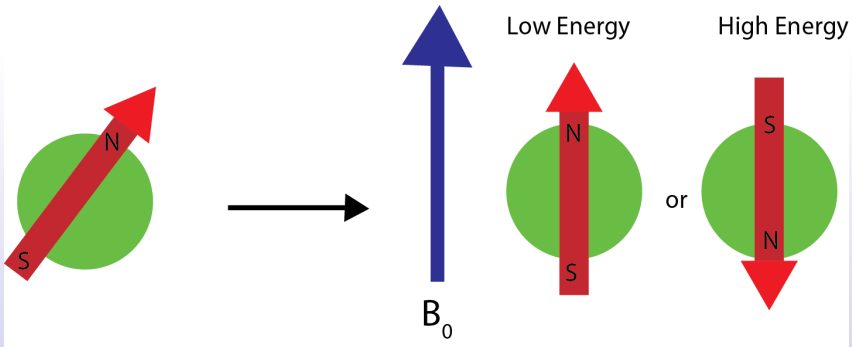

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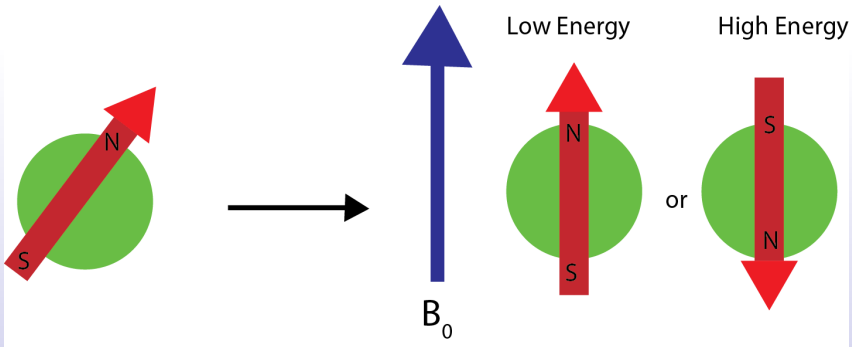
- absorption peak at $\Delta E = \hbar\omega_{res}$
- ω_{res} depends on $B_{eff}(observednucleus)$



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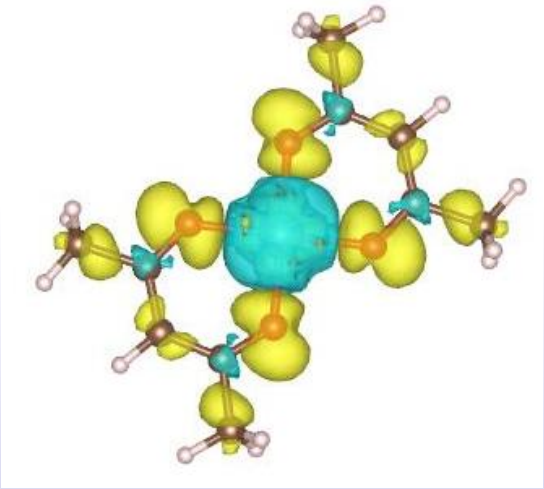

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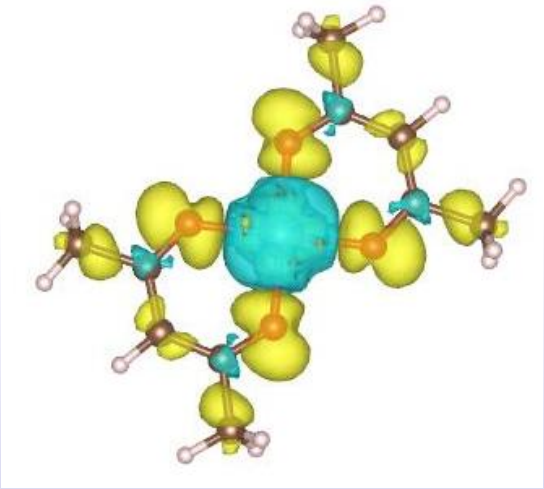

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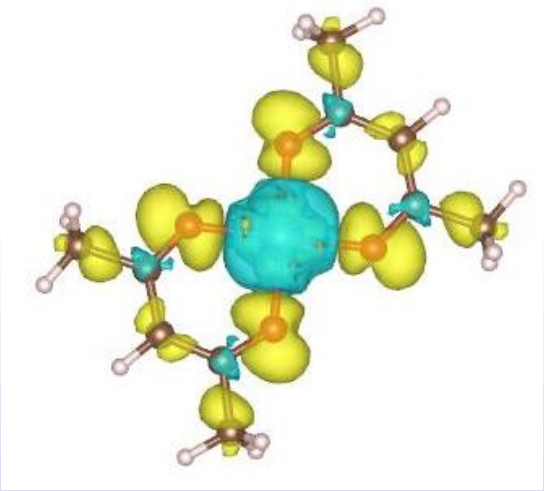

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Total shift tensor $\underline{\underline{\sigma}}$ is defined by:

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Two sources of chemical shifts:

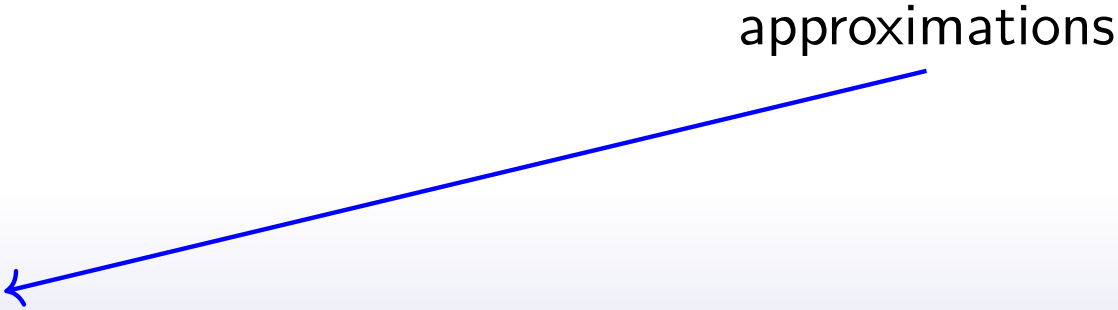
- electron density change caused by applied external magnetic field
- depends on electron density $n(\vec{r})$
- coupling between unpaired electron and observed nuclei
- depends on spin density $n_{\uparrow}(\vec{r}_{nuclei}) - n_{\downarrow}(\vec{r}_{nuclei})$

Calculation of NMR parameters:

accurate electronic wave function needed!

electronic wave function calculation

- direct solution of coupled pde not feasible
- at a given accuracy level: time needed grows exponentially as a function of number of particles



density functional theory — DFT