

Towards Density Functional Theory on a quantum computer

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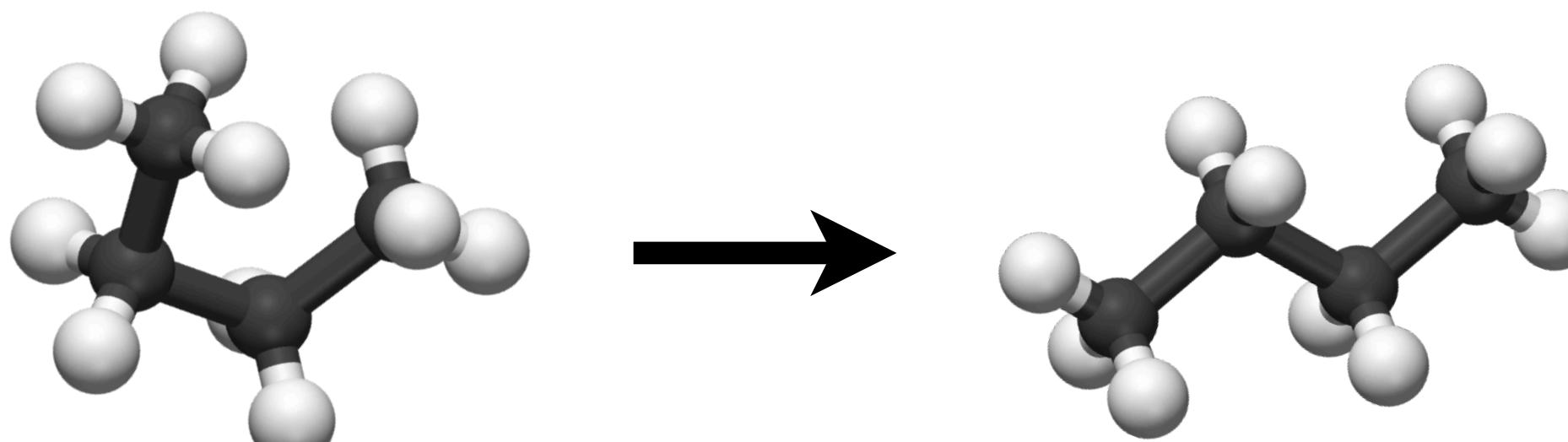


I) From Quantum chemistry to quantum computing

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What is Quantum Chemistry ?

Optimal molecular geometries



Understanding chemical reactions

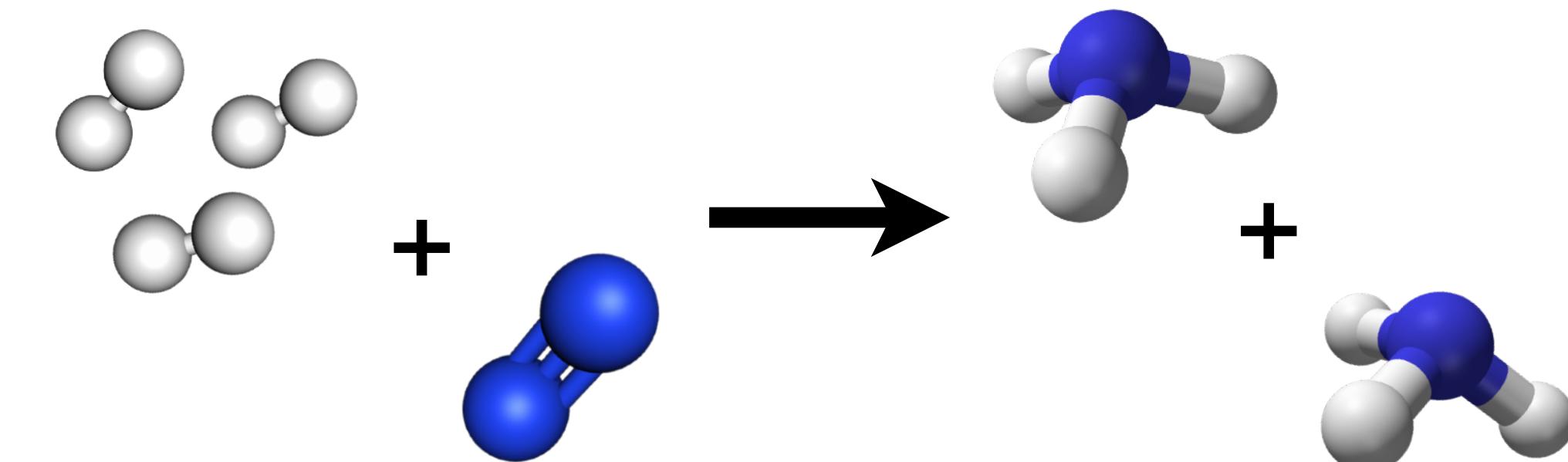
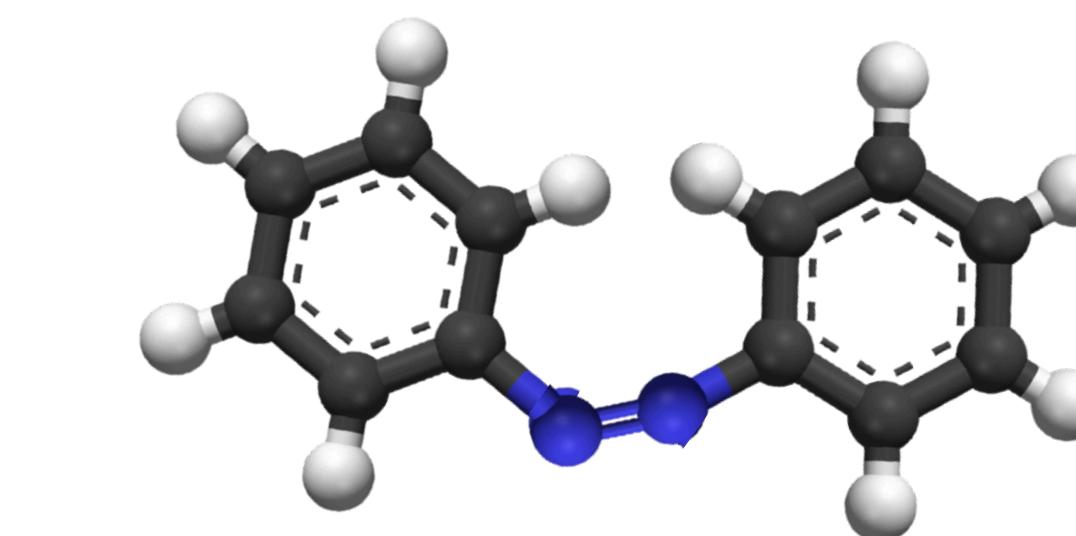
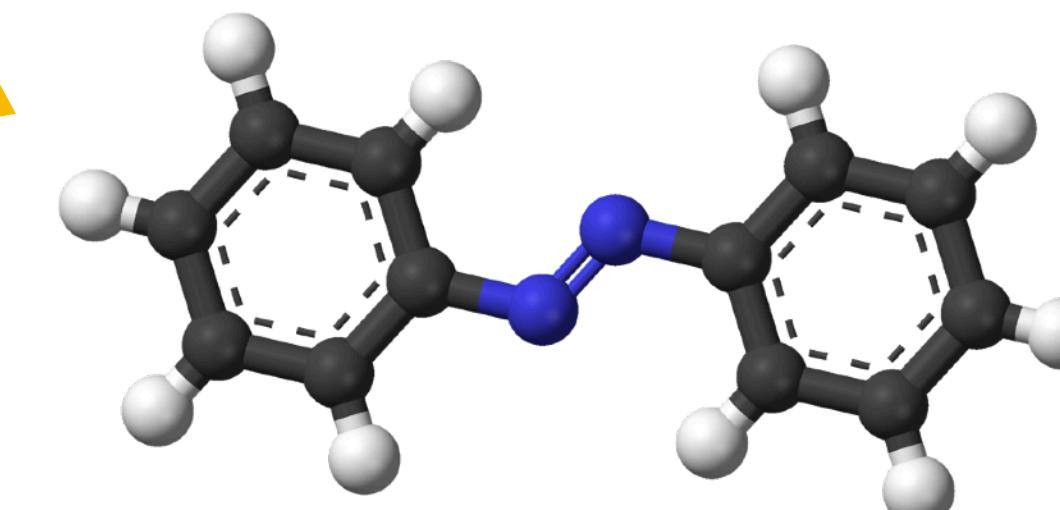
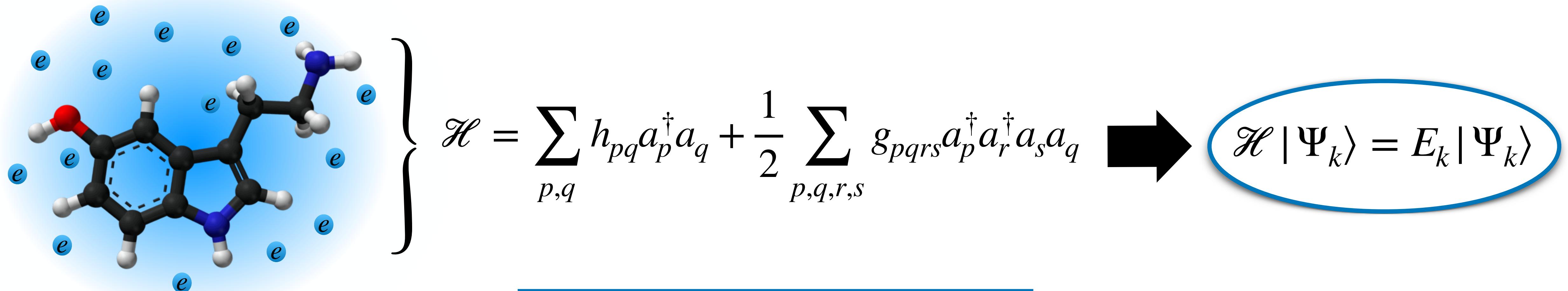


Photo-induced chemical transitions



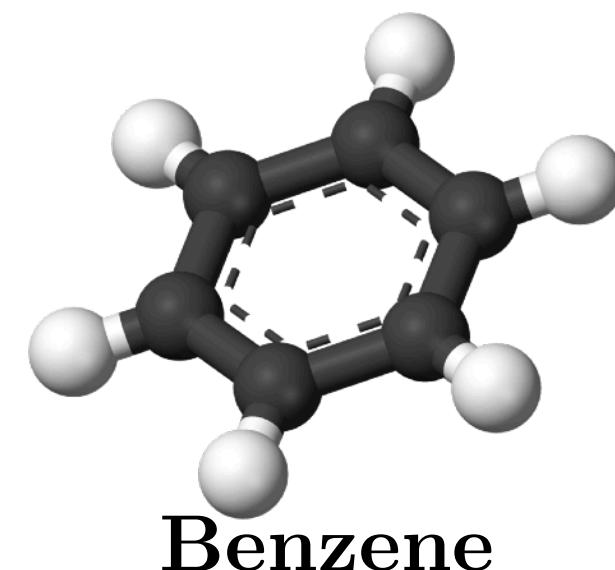
I) From Quantum chemistry to Quantum Computing

What is Quantum Chemistry ?



Wave Function Theory (WFT)

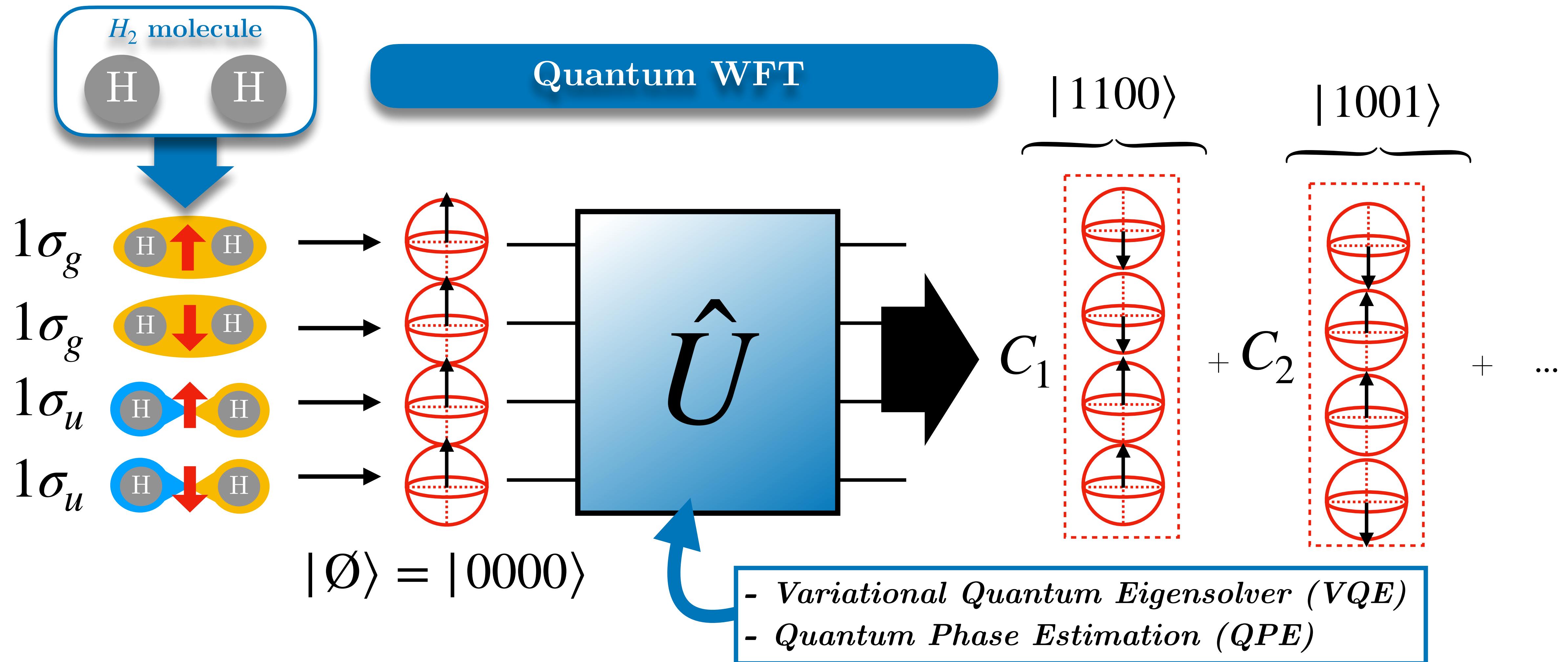
$$|\Psi_k\rangle = D_1 \underbrace{\begin{array}{c} \text{---} \\ \text{---} \\ \uparrow \quad \downarrow \end{array}}_{|1100\rangle} + D_2 \underbrace{\begin{array}{c} \text{---} \\ \text{---} \\ \uparrow \quad \downarrow \end{array}}_{|1001\rangle} + \dots$$



Observation : Ok for very small systems ...
But it scales dramatically with the size of the systems !

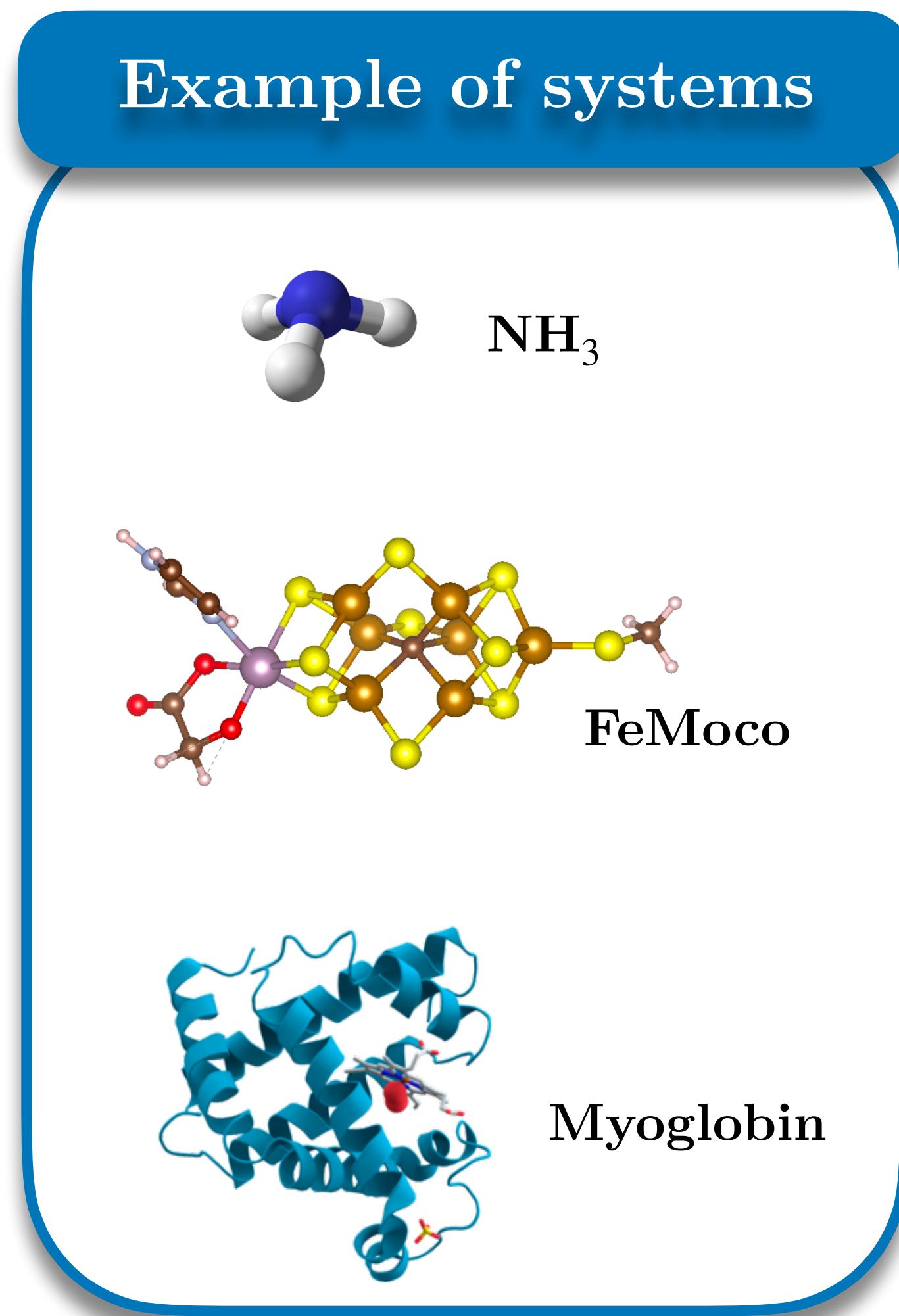
I) From Quantum chemistry to Quantum Computing

What about quantum computing ?

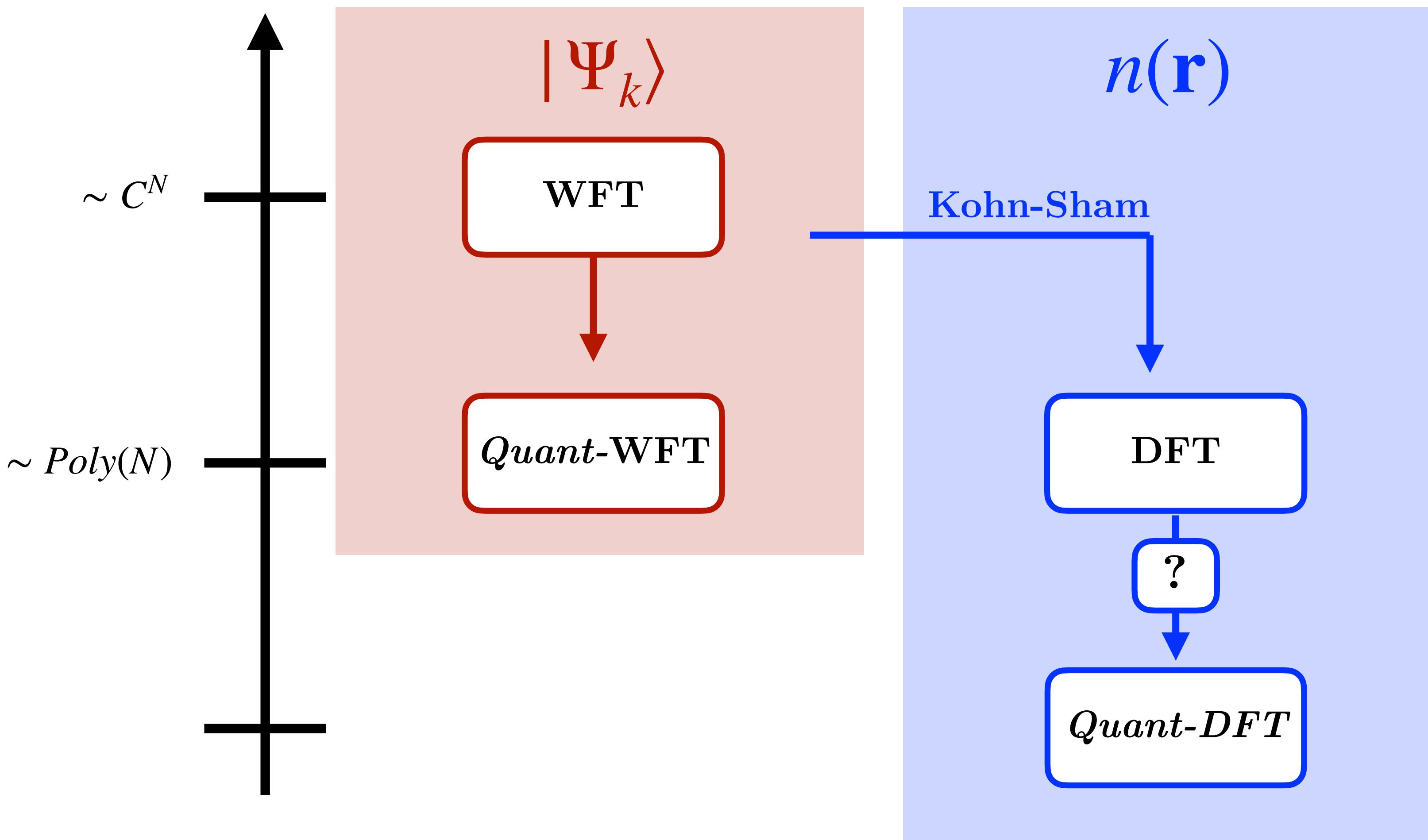


I) From Quantum chemistry to Quantum Computing

What are the motivations ?



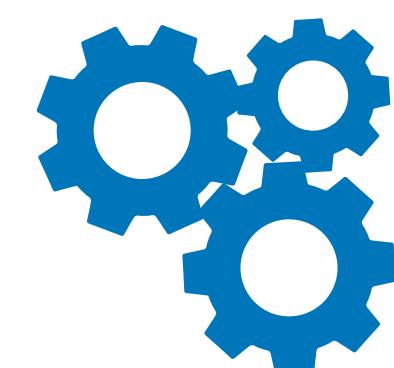
Computational cost



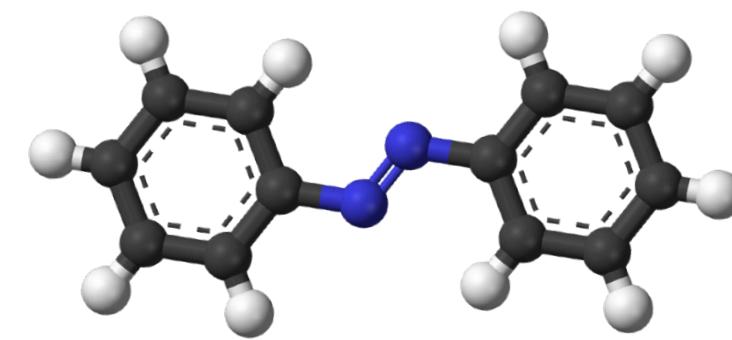
I) From Quantum chemistry to Quantum Computing

B. Senjean, S. Yalouz and M. Saubanère. [arXiv:2204.01443](https://arxiv.org/abs/2204.01443)

How does it work ?



Interacting system



$$\hat{\mathcal{H}} |\Psi_0\rangle = E_0 |\Psi_0\rangle$$

DFT = Non-interacting system

Kohn-Sham
Self-consistent
equations

$$n(\mathbf{r}) = \sum_{k=1}^{N_{elec}} |\phi_k(\mathbf{r})|^2$$

$$\hat{h}^{KS}(n(\mathbf{r}))\phi_k = \epsilon_k \phi_k$$

$$\hat{h}^{KS}(n(\mathbf{r})) = \hat{T} + \hat{v}^{KS}(n(\mathbf{r}))$$

GS energy



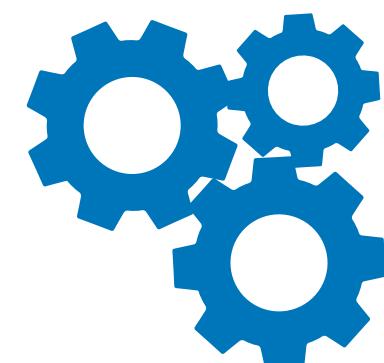
$$E_0 = \sum_k \epsilon_k + E_{Hxc}[n(\mathbf{r})] - \int \mathbf{v}^{Hxc}[n(\mathbf{r})] n(\mathbf{r}) d\mathbf{r}$$

II) Quantum algorithm for DFT

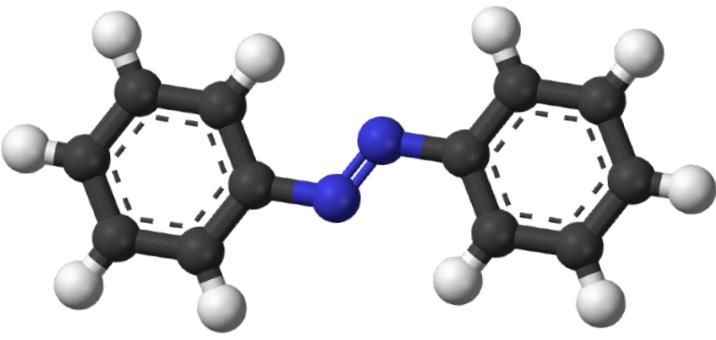
II) Quantum algorithm for DFT

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How does it work ?



Molecular system



$$\hat{h}^{KS}(n(\mathbf{r})) = \hat{T} + \hat{v}^{KS}(n(\mathbf{r}))$$

$$n(\mathbf{r}) = \sum_{k=1}^{N_{elec}} |\phi_k(\mathbf{r})|^2$$

Counter intuitive Mapping

$$\mathbf{h}^{KS}_{i,j} = \langle \chi_i | \hat{h}^{KS} | \chi_j \rangle$$

$$\begin{aligned} \{ |\chi_I\rangle \} &\rightarrow \{ |CB_I\rangle \} \\ \chi_0 &\rightarrow |000\rangle \\ \chi_1 &\rightarrow |001\rangle \\ \chi_2 &\rightarrow |010\rangle \\ \chi_3 &\rightarrow |011\rangle \\ \chi_4 &\rightarrow |100\rangle \\ \chi_5 &\rightarrow |101\rangle \\ \chi_6 &\rightarrow |110\rangle \\ \chi_7 &\rightarrow |111\rangle \end{aligned}$$

$$N_{qubit} = \log_2(N_{orb}) \rightarrow 8 \text{ MO} = 3 \text{ qubits}$$

$$\hat{H}^{aux,int} = \sum_{IJ} \mathbf{H}_{I,J}^{aux,int} |CB_I\rangle\langle CB_J|$$

State-Averaged VQE

$$|CB_I\rangle \xrightarrow{\hat{U}(\vec{\theta})} |\phi_I(\vec{\theta})\rangle = \hat{U}(\vec{\theta})|CB_I\rangle$$

$$MEASURES \left\{ \langle \phi_I(\vec{\theta}) | \hat{H}^{AUX.INT} | \phi_I(\vec{\theta}) \rangle \right\}_{I=1}^{N_e}$$

$\vec{\theta}$
Optimisation cycle

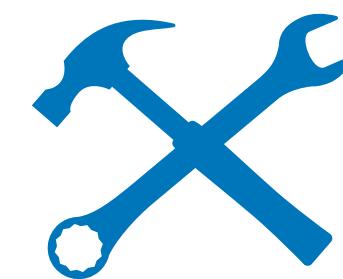


State-averaged energy cost function

$$E^{SA-VQE}(\vec{\theta}) = \sum_I^N \langle \phi_I(\vec{\theta}) | \hat{H}^{AUX.INT} | \phi_I(\vec{\theta}) \rangle$$

II) Quantum algorithm for DFT

Example

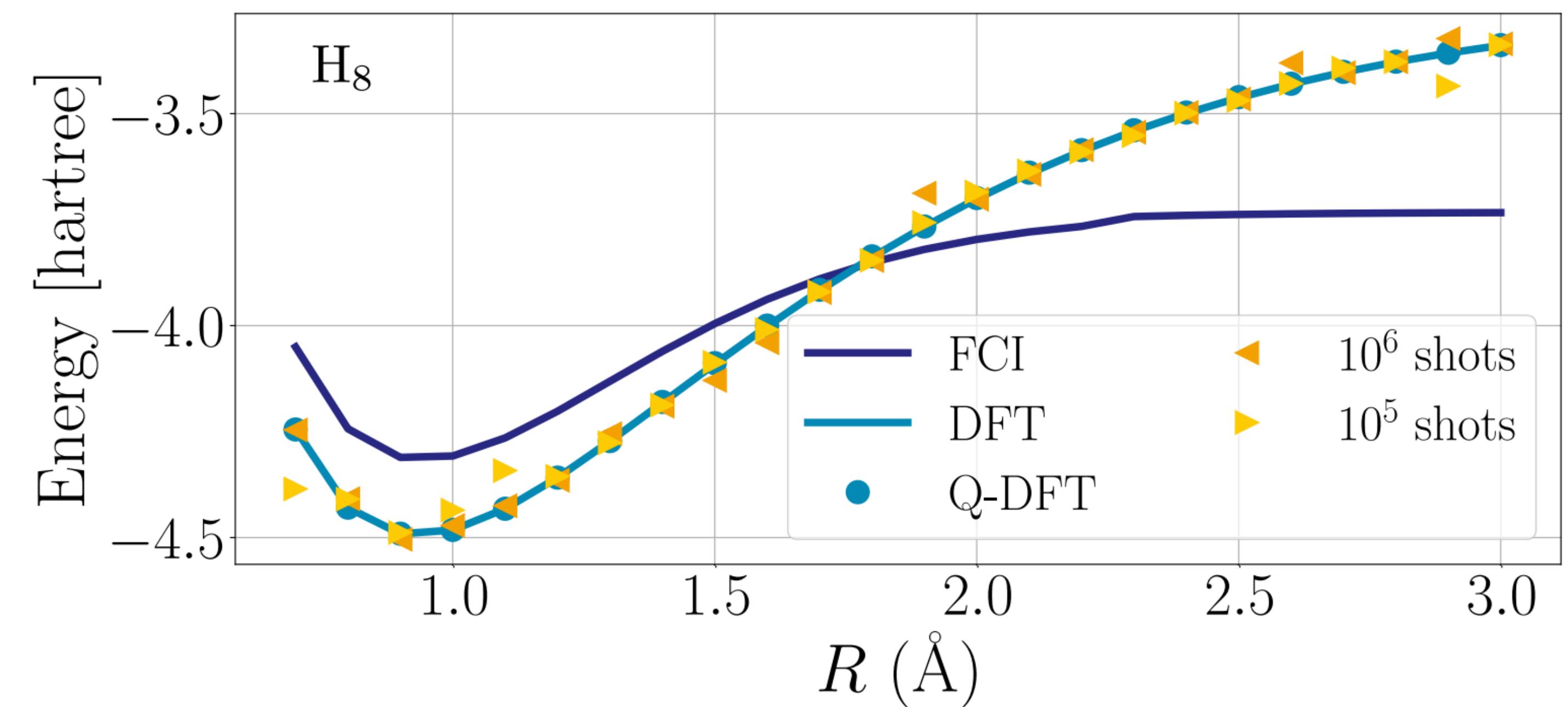
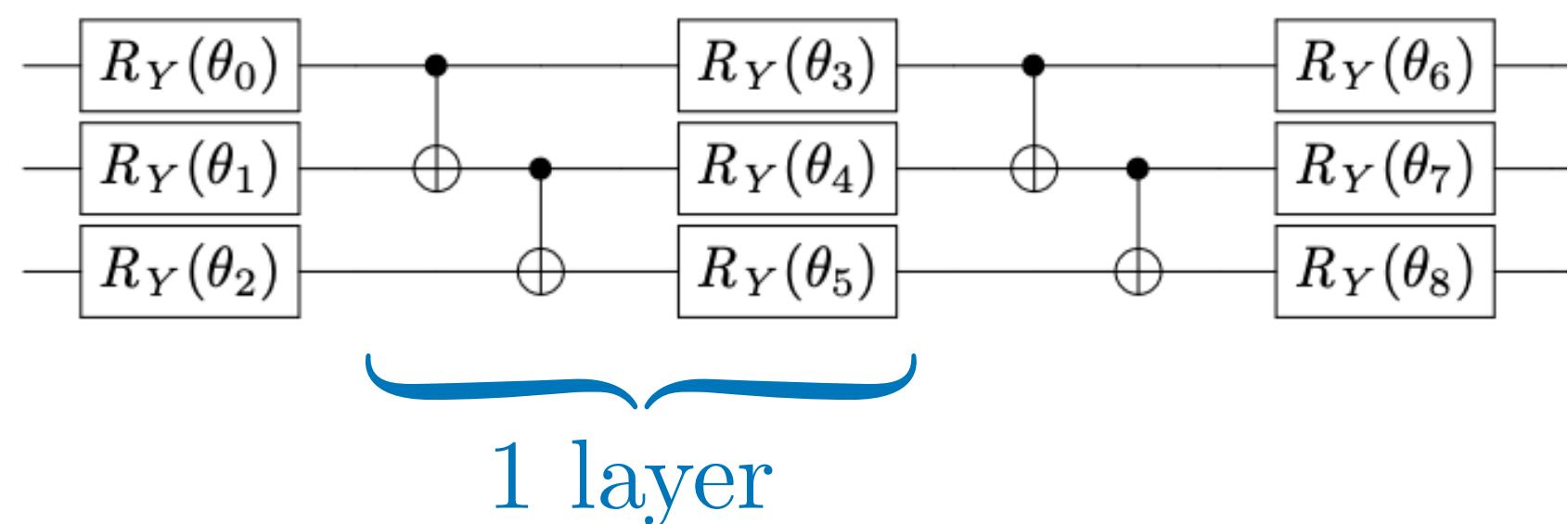


hydrogen chain with 8 atoms

Setup :

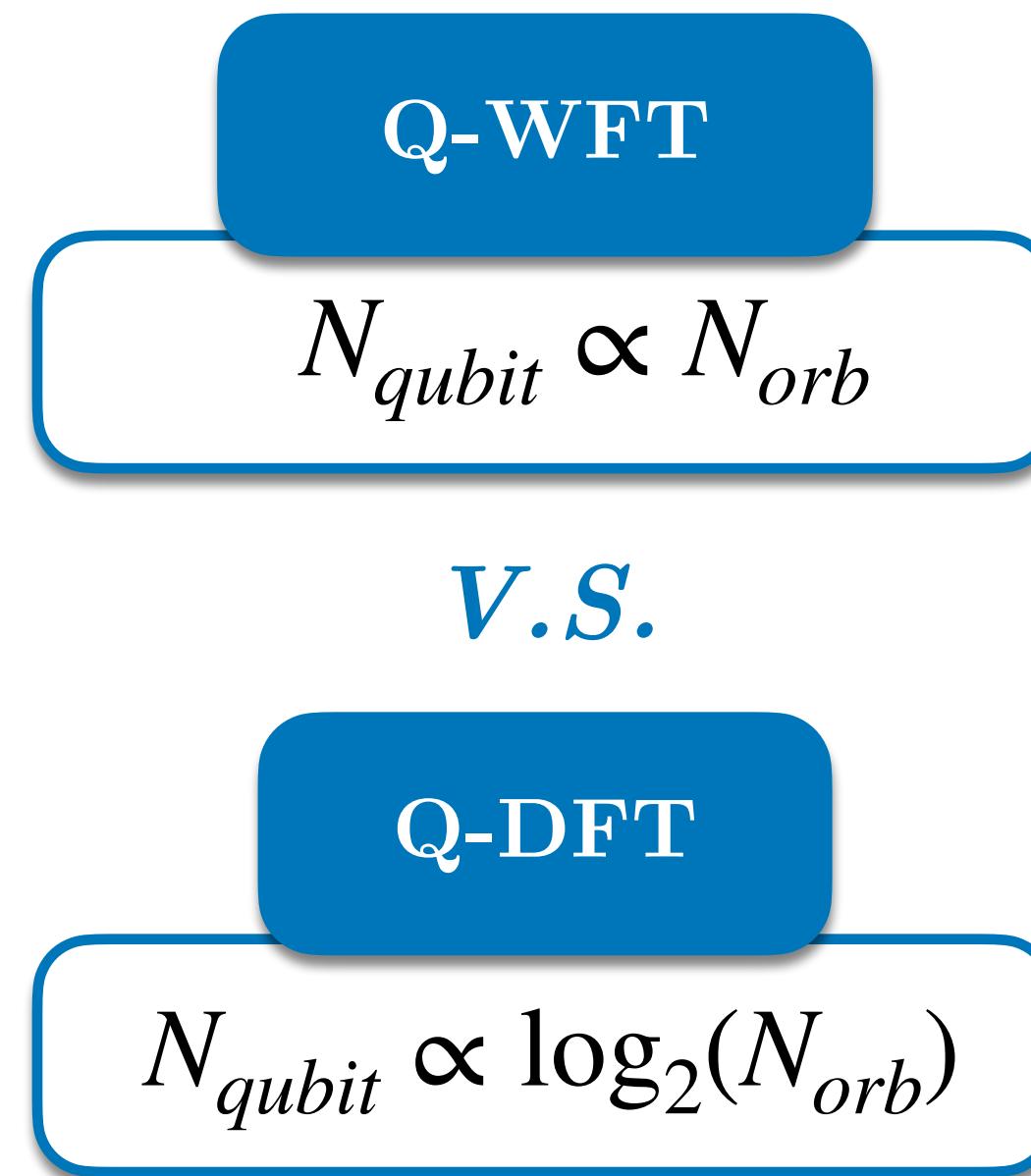
- ▶ STO-3g basis
- ▶ LDA functional
- ▶ Optimiser = SPSA
- ▶ 4 layers of ansatz (15 parameters)

$CNOT - R_Y$ ansatz

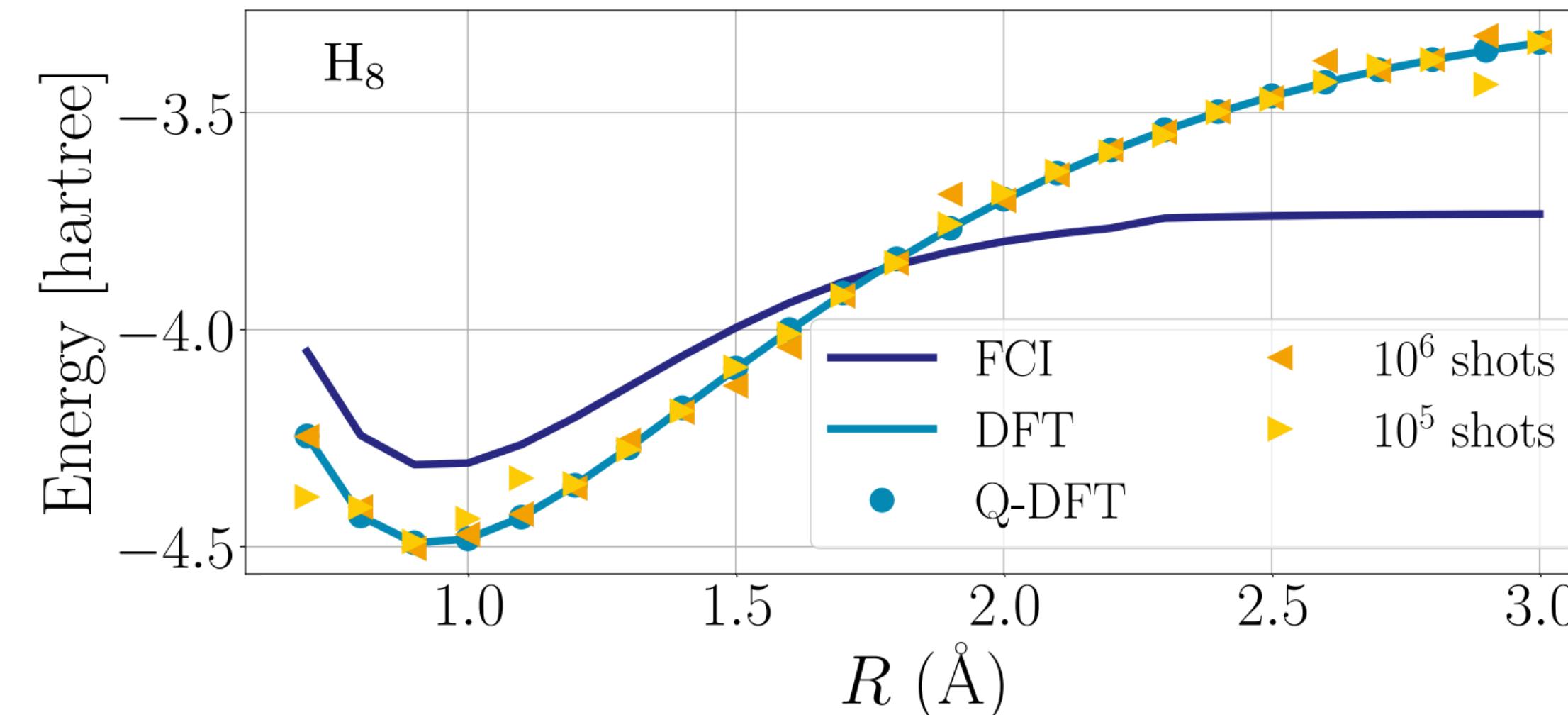


Conclusions

New paradigm



Description of ground state PES



B. Senjean, S. Yalouz and M. Saubanère. [arXiv:2204.01443](https://arxiv.org/abs/2204.01443)

What about a fault tolerant version of this algorithm ?

Thanks for your attention !

