VOLKSWAGEN

AKTIENGESELLSCHAFT

Material simulation on D-Wave

Qubits Europe 2018, Munich

12.04.2018 - Michael Streif

DATA:LAB MUNICH

Powered by...

Motivation

- Simulating electronic structure properties is important for different areas of research and industry
- Numerical approximations rapidly become unfeasible
- Quantum computers do not require exponentially increasing time to solve larger systems

Long term goal:

Investigating the use of quantum computers to find advanced materials

Electronic structure calculations on quantum computers

- Mainly targeted by gate model approaches
- Quantum algorithms: variational quantum eigensolver (VQE), phase estimation algorithm (PEA)
- Current gate model devices suffer from different challenges:
  - Small number of qubits
  - Decoherence effects
  - Imperfect qubits and gates

Can we instead use a quantum annealer, e.g. a D-Wave machine, for such calculations?

Yes! [1]

[1] Xia, Teng, and Kais. "Electronic Structure Calculations and the Ising Hamiltonian." *The Journal of Physical Chemistry B* (2017)

Quantum chemistry in a nutshell

- Molecules can be described by a fermionic Hamiltonian

$$H = \sum_{i,j} h_{ij}(R) a_i^\dagger a_j + \frac{1}{2} \sum_{i,j,k,l} h_{ijkl}(R) a_i^\dagger a_j^\dagger a_k a_l$$

- Jordan-Wigner transformation to map it onto a qubit Hamiltonian

$$H = \sum_{i,\alpha} h_\alpha^i \sigma_\alpha^i + \sum_{i,j,\alpha,\beta} h_{\alpha\beta}^{ij} \sigma_\alpha^i \sigma_\beta^j + \sum_{i,j,k,\alpha,\beta,\gamma} h_{\alpha\beta\gamma}^{ijk} \sigma_\alpha^i \sigma_\beta^j \sigma_\gamma^k + \dots$$

Mapping the problem onto D-Wave (1)

$$H = \sum_{i,\alpha} h^i_\alpha \sigma^i_\alpha + \sum_{i,j,\alpha,\beta} h^{ij}_{\alpha\beta} \sigma^i_\alpha \sigma^j_\beta + \sum_{i,j,k,\alpha,\beta,\gamma} h^{ijk}_{\alpha\beta\gamma} \sigma^i_\alpha \sigma^j_\beta \sigma^k_\gamma + \dots$$

- σ_x, σ_y and σ_z terms instead of σ_z terms only
- k-local terms instead of 2-local

- [1] shows how to map a n-qubit Hamiltonian with σ_x, σ_y and σ_z terms to a rn-qubit Hamiltonian with σ_z terms only

$$\sigma^i_x \to \frac{1 - \sigma_z^{i_j} \sigma_z^{i_k}}{2} S'(j) S'(k) \qquad \sigma^i_y \to \mathrm{i} \frac{\sigma_z^{i_k} - \sigma_z^{i_j}}{2} S'(j) S'(k)$$

$$\sigma^i_z \to \frac{\sigma_z^{i_j} + \sigma_z^{i_k}}{2} S'(j) S'(k) \qquad I^i \to \frac{1 + \sigma_z^{i_j} \sigma_z^{i_k}}{2} S'(j) S'(k)$$

[1] Xia, Teng, and Kais. "Electronic Structure Calculations and the Ising Hamiltonian." *The Journal of Physical Chemistry B* (2017)

Mapping the problem onto D-Wave (2)

- Reducing the dimensions from k-local to 2-local by using ancillary qubits
- Illustrative example (by [1]):

$$\min(\pm x_1 x_2 x_3) = \min(\pm x_4 x_3 + x_1 x_2 - 2x_1 x_4 - 2x_2 x_4 + 3x_4)$$
$$x_1, x_2, x_3, x_4 \in \{0, 1\}$$

- Ising representation:

$$H = \sum_i h'_i \sigma_z^i + \sum_{i,j} J'_{ij} \sigma_z^i \sigma_z^j$$

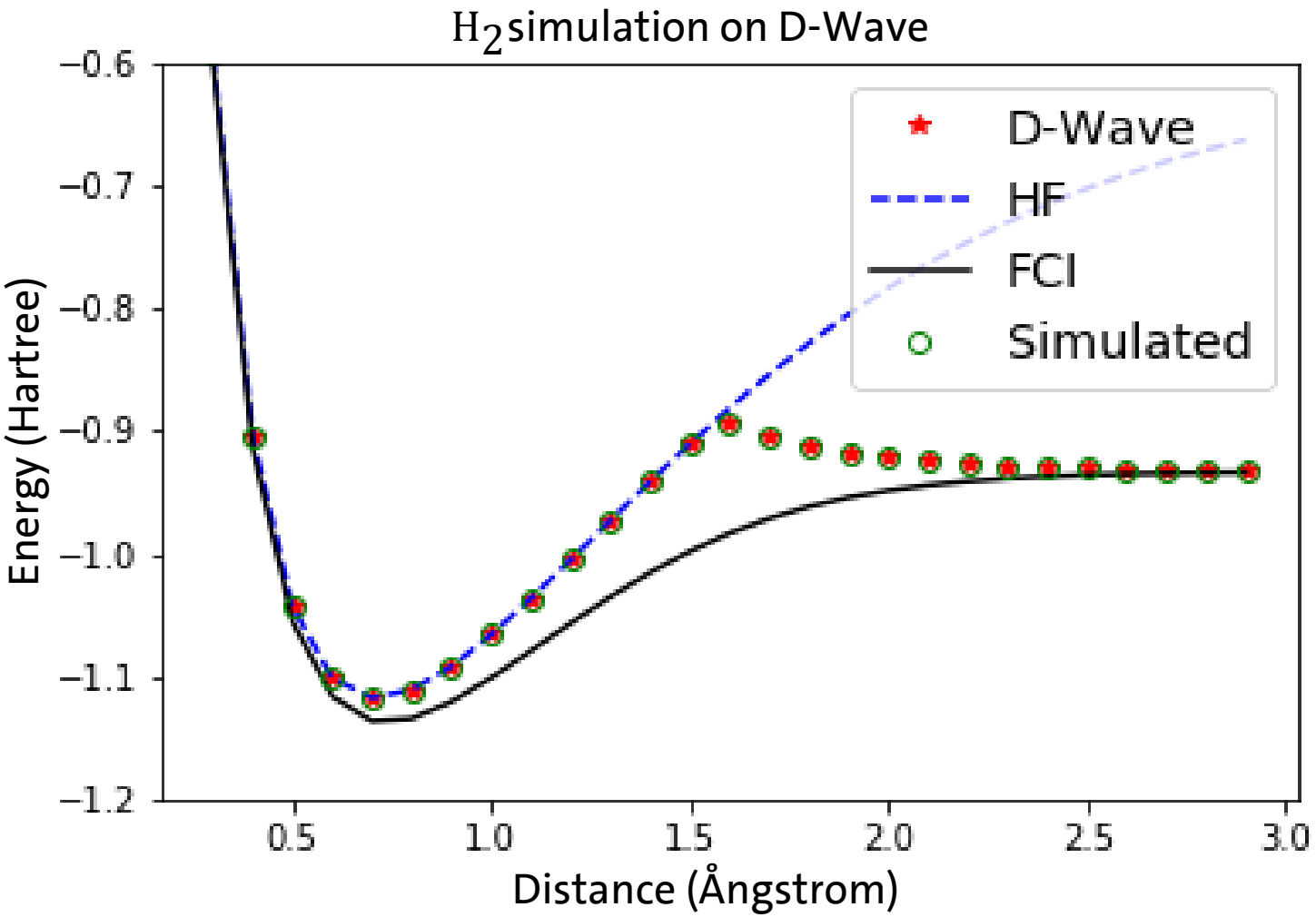
[1] Xia, Teng, and Kais. "Electronic Structure Calculations and the Ising Hamiltonian." *The Journal of Physical Chemistry B* (2017)

Experiments on D-Wave

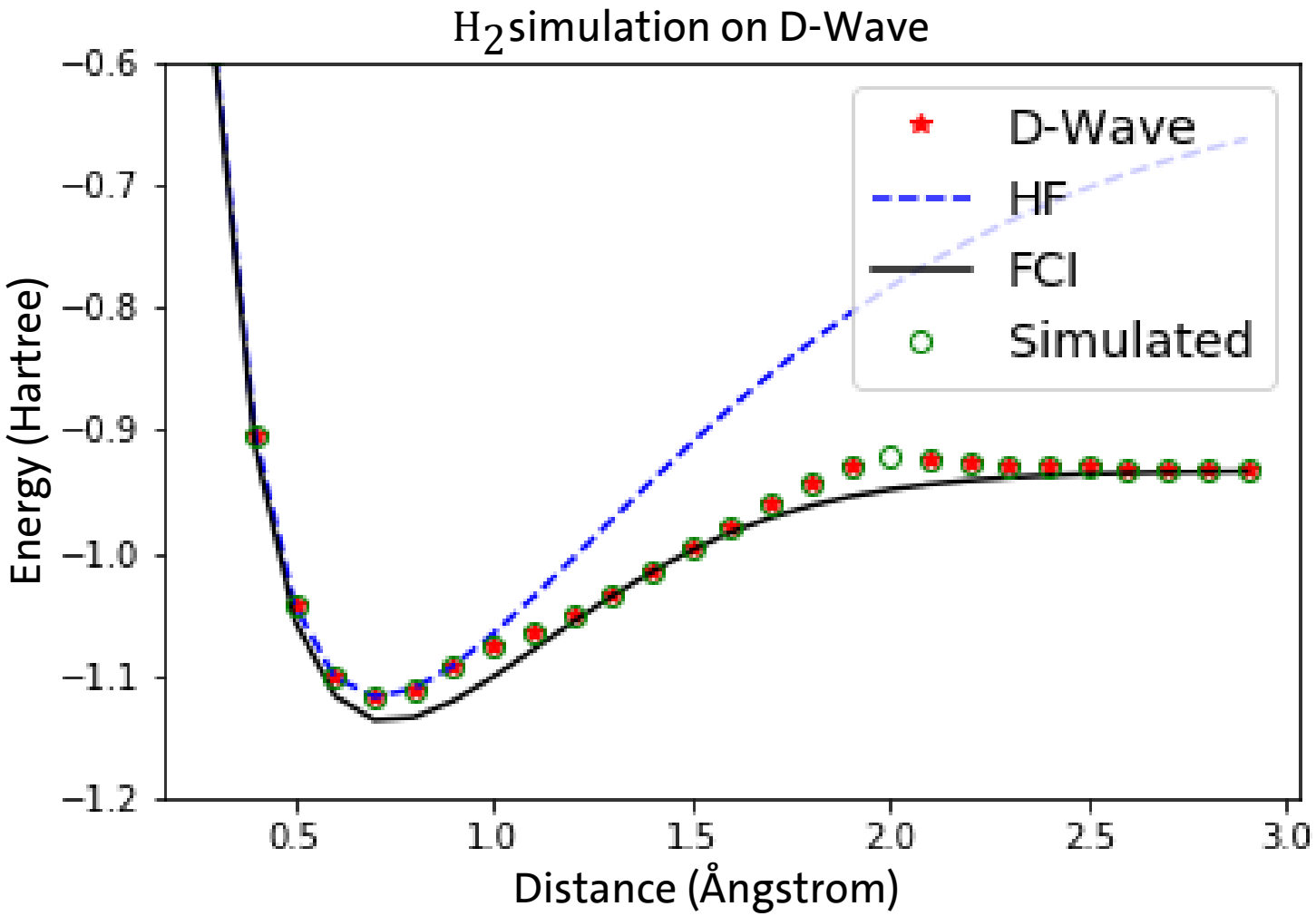
- Molecular hydrogen, H_2 (2 electrons)
- Lithium hydride, LiH (4 electrons)

1. Calculate the fermionic Hamiltonian for a chosen basis set
2. Map onto an Ising Hamiltonian for a specific accuracy parameter r
3. Comparison to numerical calculations, as Hartree-Fock (HF) or Full Configuration Interaction (FCI)

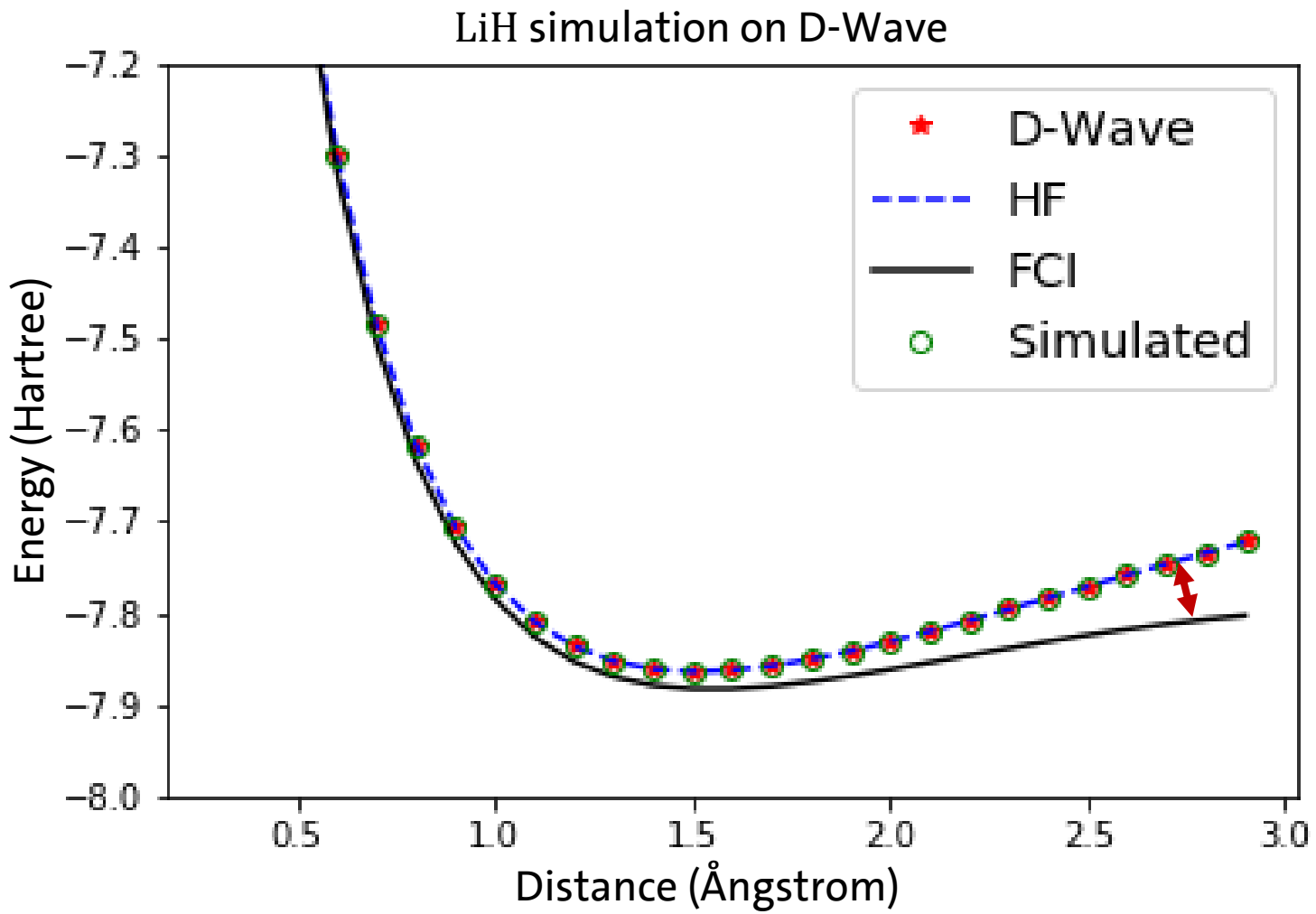
Results – H_2 Molecule – $r = 2$



Results – H_2 Molecule – $r = 4$



Results – LiH Molecule – $r = 2$



Take home message

- It is possible to use a D-Wave machine for electronic structure calculations

Outlook

- Improve the results by increasing the accuracy parameter r
- Study the scaling behavior for larger systems
- Find new approaches for larger molecules and implement these on a D-Wave quantum computer

Thank you.

Any questions?