Reference-State Error Mitigation:
A Strategy for High Accuracy Quantum Computation of Chemistry

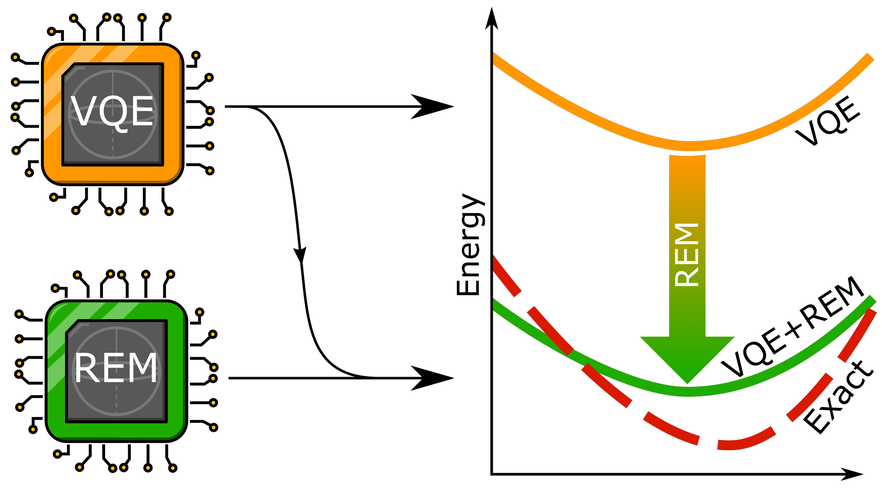
Werner Dobrautz[a,*], Mårten Skogh[a,b], Phalgun Lolur[a], Christopher Warren[c], Janka Biznárová[c], Amr Osman[c], Giovanna Tancredi[c], Goran Wendin[c], Jonas Bylander[c], Martin Rahm[a]

[a] Department of Chemistry and Chemical Engineering, Chalmers University of Technology, Sweden
[b] Data Science & Modelling, Pharmaceutical Science, R&D, AstraZeneca, Gothenburg, Sweden
[c] Department of Microtechnology and Nanoscience MC2, Chalmers University of Technology, Sweden

dobrautz@chalmers.se

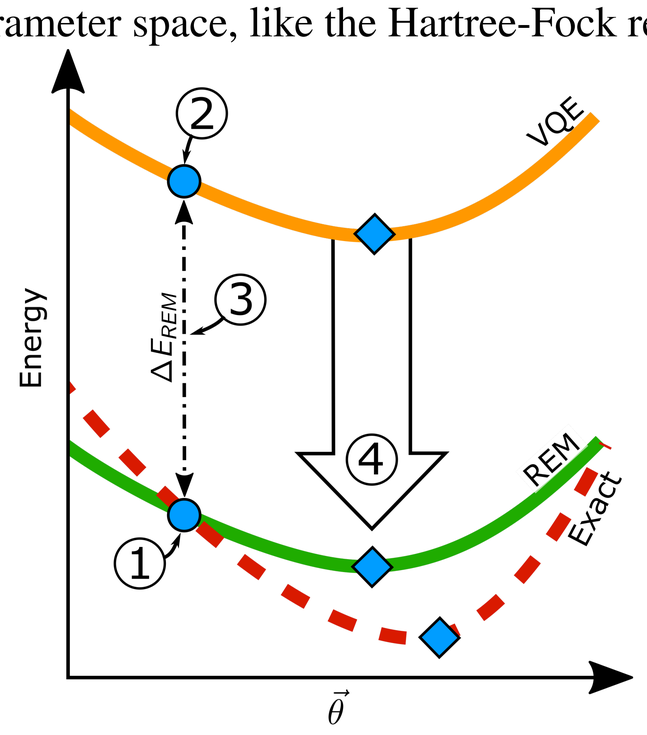
Overview

- Quantum computers are limited by decoherence and gate errors[1]
- Reference-state error mitigation (REM)[2] can be implemented on current and near-term, requires **minimal postprocessing** and can be applied alongside existing mitigation procedures
- The **method is Ansatz-agnostic** and is compatible with various variational quantum algorithms like the VQE[3] or VarQITE[4]
- REM demonstrated **significant improvement in the computational accuracy** of ground state energies of small molecules (H_2, HeH^+, and LiH) on superconducting quantum hardware
- Simulations of noisy circuits demonstrate the **method's scalability**



Reference-state Error Mitigation

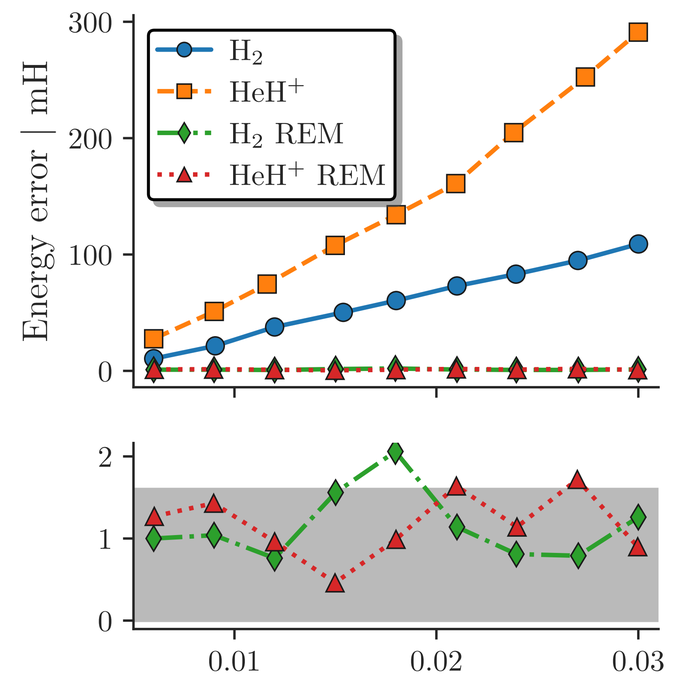
We take advantage of classically tractable and easy-to-prepare points in the VQE parameter space, like the Hartree-Fock reference state.



1. Classically compute exact reference energy (i.e. Hartree-Fock), $E(\boldsymbol{\theta}_{\text{ref}})$
2. Measure reference energy on noisy device $\mathcal{E}(\boldsymbol{\theta}_{\text{ref}})$, with reference parameters $\boldsymbol{\theta}_{\text{ref}}$
3. Calculate REM correction: $\Delta E_{\text{REM}} = \mathcal{E}(\boldsymbol{\theta}_{\text{ref}}) - E(\boldsymbol{\theta}_{\text{ref}})$
4. Correct final VQE energy with REM correction

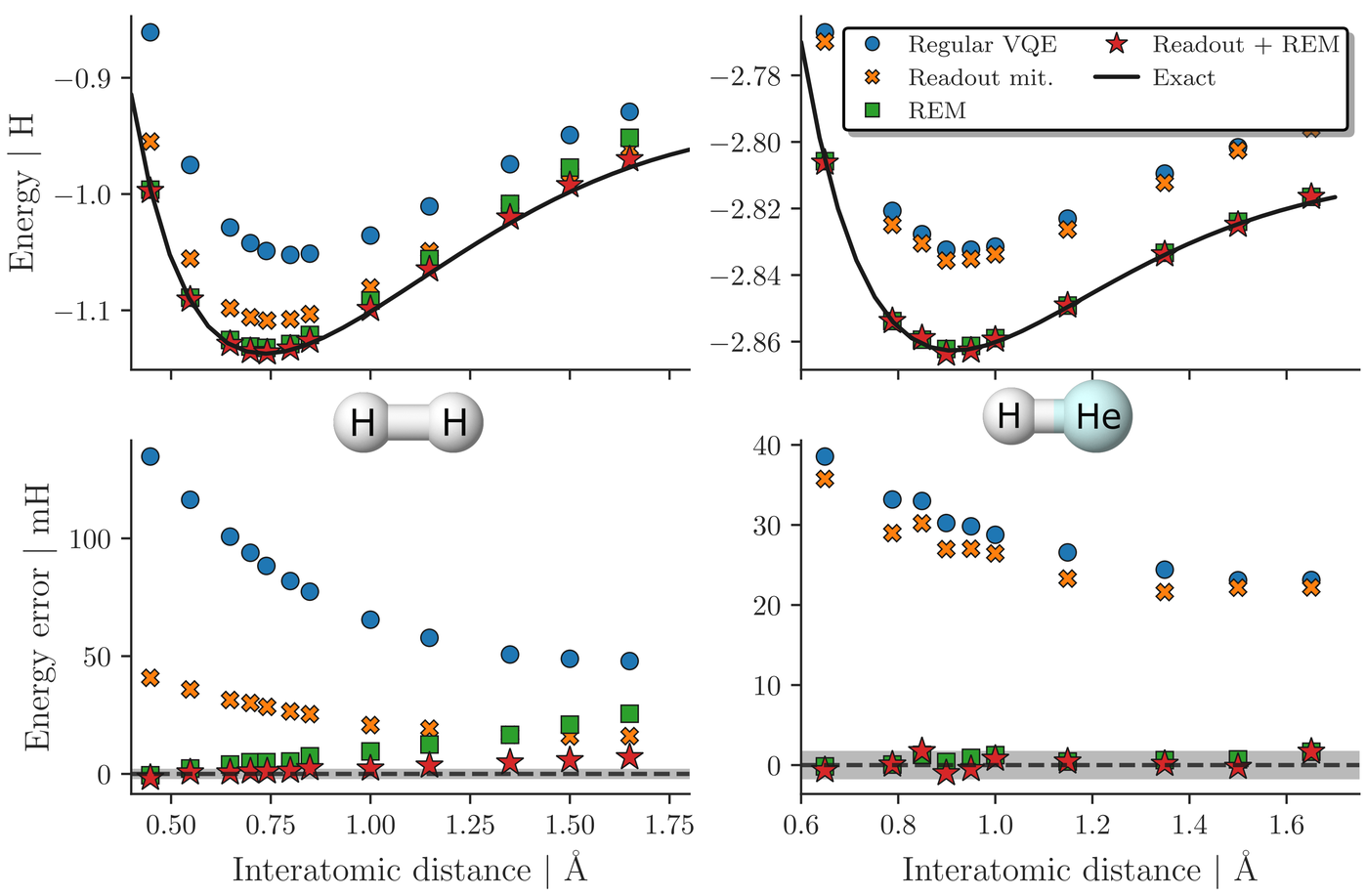
Noise-resilience

REM is noise-resilient: effective despite the steady increase in single- and two-qubit depolarizing error rates.



Results

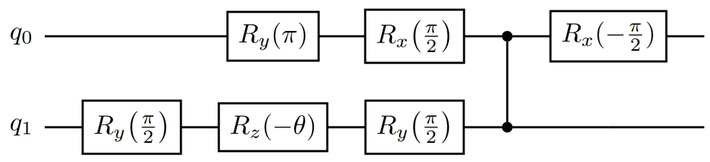
Significant improvement in the computational accuracy of ground state energies of small molecules (H_2, HeH^+, LiH and BeH_2) on superconducting quantum hardware



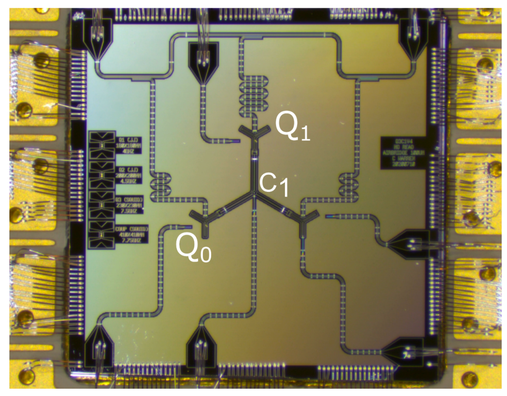
Molecule	$\Delta E_{\text{error,VQE}}$	$\Delta E_{\text{error,REM}}$	Ansatz	Qubits	Two-qubit Gates
H_2	0.029(6)	0.002(8)	Hardware-efficient	2	1
HeH^+	0.029(4)	0.003(6)	Hardware-efficient	2	4
LiH	0.288(33)	0.029(26)	Hardware-efficient	4	6
BeH_2	1.605(5)	0.0263(10)	UCCSD	6	1096

Hardware

Hardware-efficient Ansatz[5] for H_2:



First quantum chemistry calculation on Chalmers Särimner device.



References

[1] Nielsen, M., & Chuang, I. (2010). Quantum Computation and Quantum Information, Cambridge University Press.
[2] P. Lolur, , M. Skogh, **W. Dobrautz**, C. Warren, J. Biznárová, A. Osman, G. Tancredi, G. Wendin, J. Bylander, and M. Rahm*, J. Chem. Theory Comput. 2023, **19**, 3, 783
[3] Peruzzo, A., *et al.*, Nat. Commun. **5**, 4213
[4] McArdle, S., Jones, T., Endo, S. *et al.*, npj Quantum Inf. **5**, 75
[5] Kandala, A., *et al.*, Nature **549**, 242