CIFellows 2020-2021

Computing Innovation Fellows

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Describing Chemical Dynamics with Quantum Simulators

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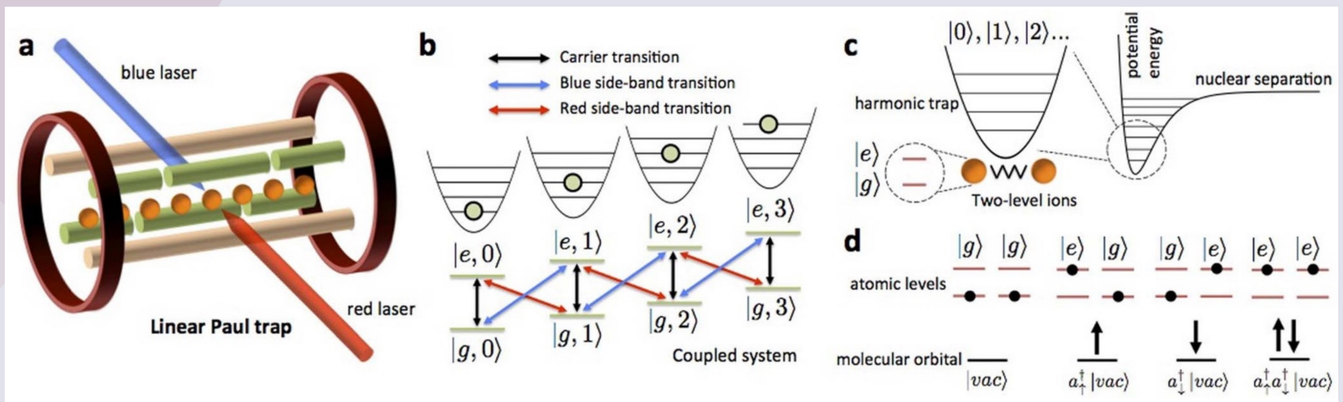
Quantum simulations with trapped ions

- Simulating molecules with numerical methods are only applicable to small molecules in a limited parameter regime.
- Trapped-ion systems are a promising platform for quantum computation and quantum simulations.
- We have used trapped-ion systems to study charge flow in molecules



Simulating quantum chemistry with trapped-ion systems. Retrieved from Yung, M-H., et al. *Sci. Rep.* 4.1 (2014): 1-7.

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Mapping molecules to trapped ions

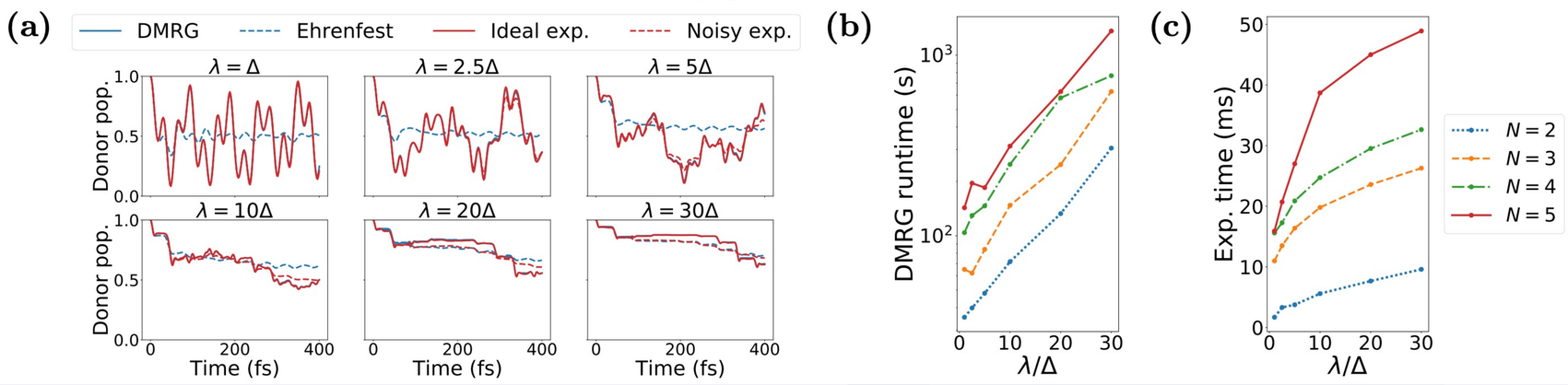
- Molecules are commonly described by mathematical expressions known as Hamiltonians.
- The molecular Hamiltonians can be mapped to trapped-ion Hamiltonians to perform exact simulations of chemical processes.

$$\hat{H}_{\mathrm{mol}} = \sum_{i,j=1}^{M} \frac{\Omega_{i,j}}{2} \hat{\psi}_i^\dagger \hat{\psi}_j \left(1 + \sum_{k=1}^{N} \eta_{i,j,k}(\hat{a}_k + \hat{a}_k^\dagger)\right) + \sum_{k=1}^{N} \nu_k \hat{a}_k^\dagger \hat{a}_k \longrightarrow \hat{H}_{\mathrm{TI}} = \frac{\tilde{\Omega}}{2}\left[\hat{\sigma}_+ \left(1 + \sum_{k=1}^{N} \tilde{\eta}_k(\hat{b}_k + \hat{b}_k^\dagger) e^{i(\phi - \delta t)}\right) + h.c.\right] + \sum_{k=1}^{N} \tilde{\nu}_k \hat{b}_k^\dagger \hat{b}_k$$

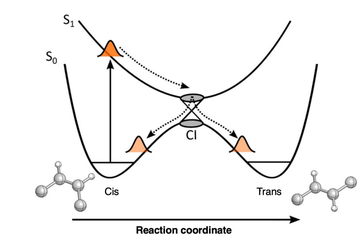
Quantum simulations

- We have compared the performance of trapped-ion quantum simulations with two classical algorithms, tDMRG and Ehrenfest, by simulating the dynamics of a toy model system.
- Quantum simulators reduce the required simulation time.

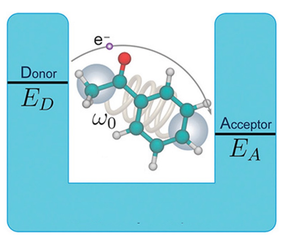
$$\hat{H}_{\mathrm{toy}} = \frac{\Delta}{2}\left(|D\rangle\langle A| + |A\rangle\langle D|\right) + \sum_{k=1}^{N}\left[\kappa\left(|D\rangle\langle D| - |A\rangle\langle A|\right)\left(\hat{a}_k + \hat{a}_k^\dagger\right) + \nu_k \hat{a}_k^\dagger \hat{a}_k\right]$$



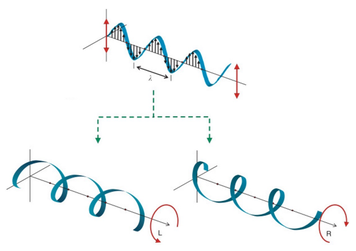
Chemical problems to study



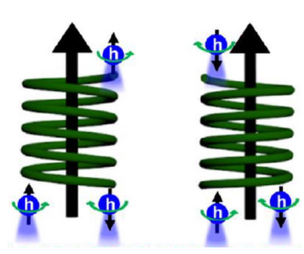
Conical intersections



Vibrationally-assisted ET



Polarized light ET



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