National Academies Consensus Study:
Guiding Research Directions in Chemistry & QIS

Select Takeaways from Report:
- Report identifies major fundamental research directions for chemistry and QIS in both near-term and long-term.
- Urges for more cross-diciplinary collaborations.
- Highlights need for more infrastructure development.
- Emphasizes the need for workforce development, in particular, expansion of technical skillset, inclusion of diverse backgrounds, and increase of permanent staff.

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https://nap.nationalacademies.org/catalog/26850/advancing-chemistry-and-quantum-information-science-an-assessment-of-research

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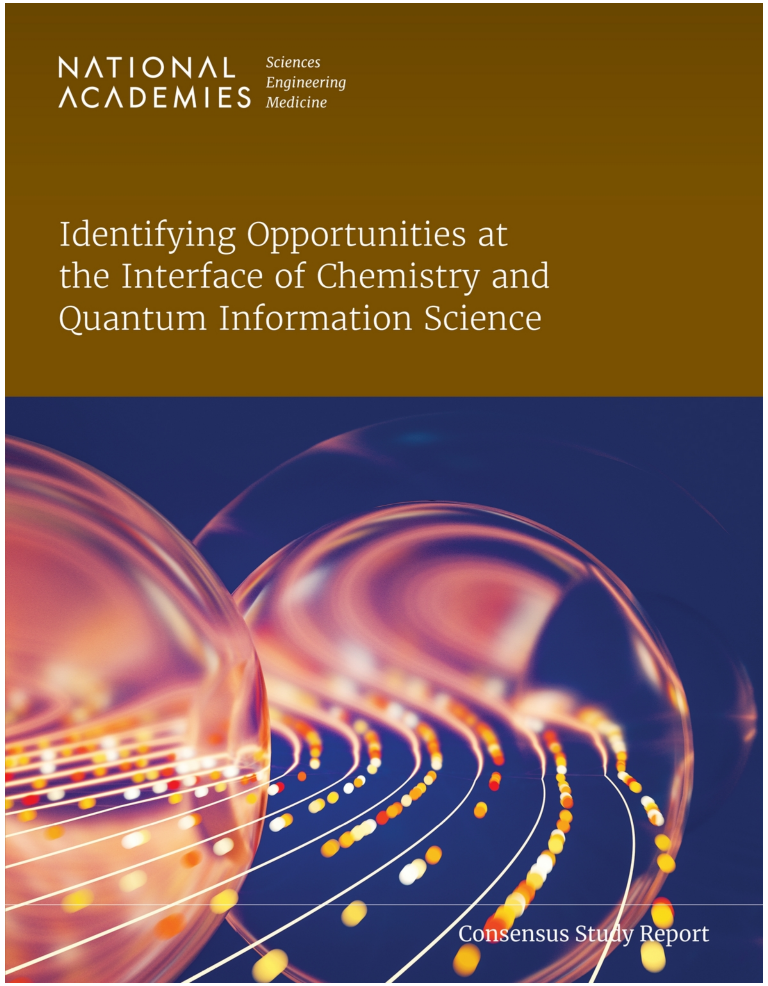

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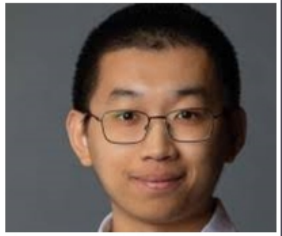

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Select Research Priorities: Measurement and Control of Molecular Quantum Systems (Chapter 3)

Develop new approaches and techniques for addressing and controlling multiple electron and nuclear spins and optical cycling centers in molecular systems.

Develop techniques to probe molecular qubits at complex interfaces to inform their systematic control.

Develop enhanced spectroscopic and microscopic techniques by creating

i. entangled photon sources with higher yield and better spectral coverage, and

ii. high-finesse cavities and nanophotonics for molecular qubit systems.

Develop and exploit alternative approaches to spin polarization and coherence control (e.g., chirality-induced spin selectivity and electric field effects).

Use molecular systems to teleport quantum information over distances greater than 1 μm with high fidelity.

Develop molecular quantum transduction schemes that take advantage of entangled photons as well as entangled electrons and nuclear spins.

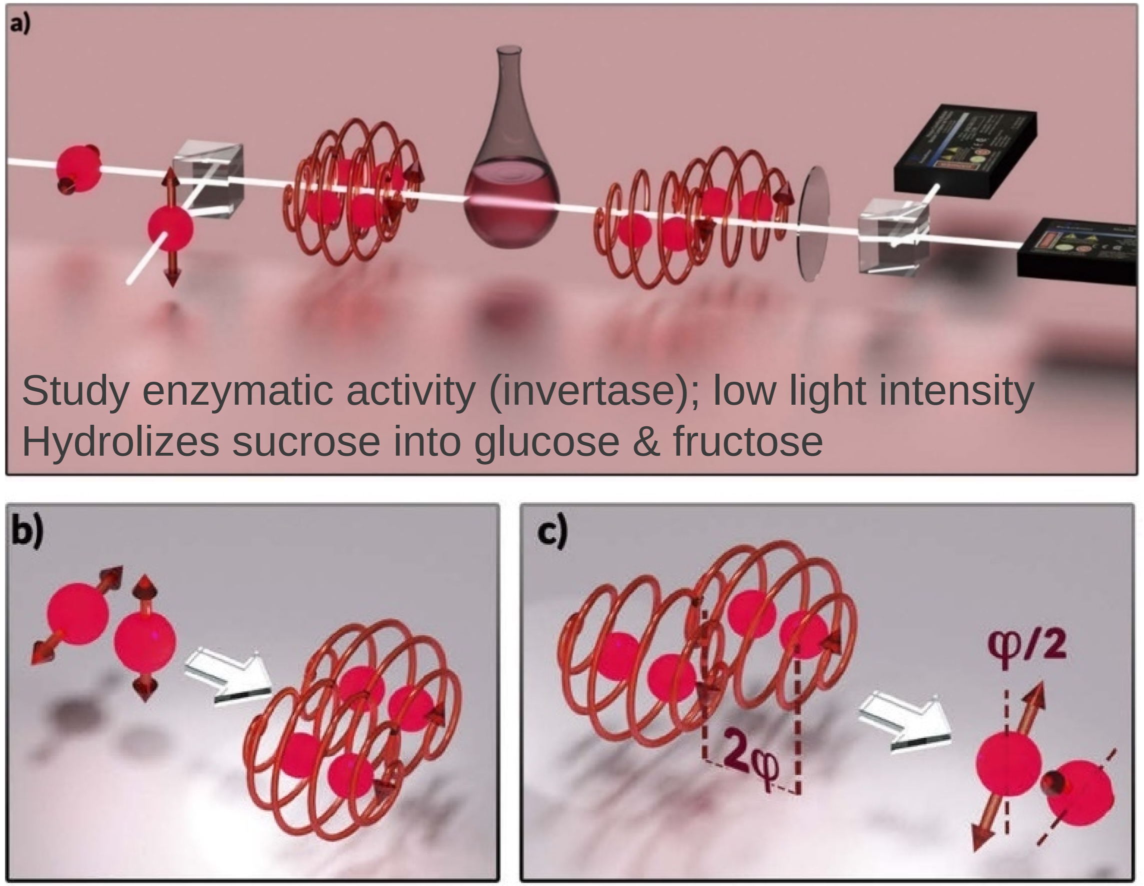
Advance quantum sensing techniques to further understand biological systems.

Use bio-inspired quantum processes for the development of new quantum technologies.

Provide broadly accessible state-of-the-art measurement techniques and instrumentation for the chemistry community to accomplish all of the above goals.

Develop Enhanced Quantum Spectroscopy/Microscopy

Tracking enzymatic reactions with quantum light

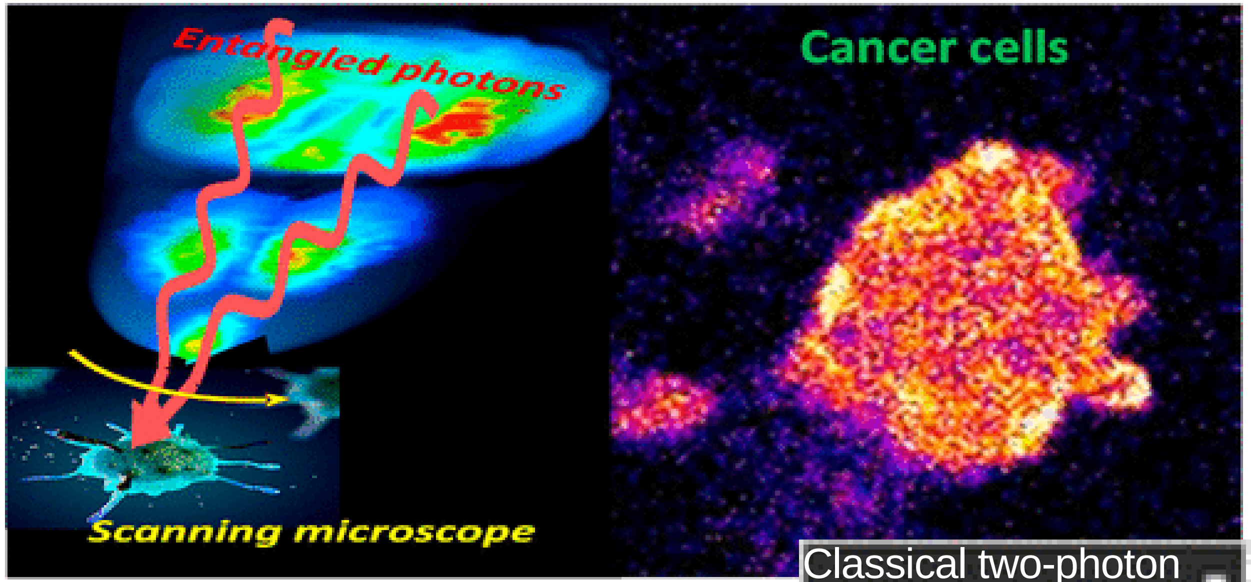


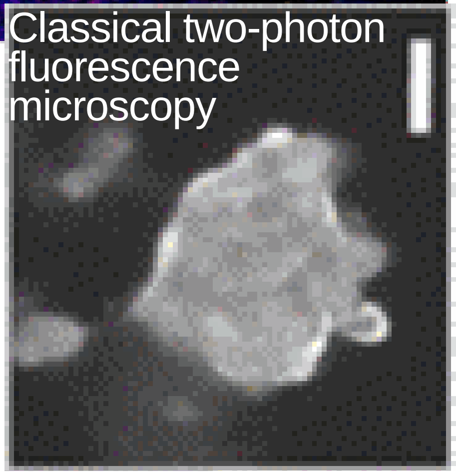
- Exploit coherent superposition (N00N) of SPDC pairs:

$$|\psi\rangle = \hat{a}_H^\dagger \hat{a}_V^\dagger |0\rangle = \frac{1}{\sqrt{2}}\left(|2_R 0_L\rangle - |0_R 2_L\rangle\right)$$

Cimini et al., Optics Express **27**, 35245 (2019)

Quantum light-enhanced two-photon imaging





- Entangled photons via spontaneous parametric down-conversion (SPDC)
- Enhanced two-photon absorption compared to classical (random) light
- Allows for much lower excitation intensity compared to classical light
- ~10^7 photons/s (×10^{-6} classical light)

Varnavski et al., J. Phys. Chem. Lett. **13**, 2772 (2022)

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Recommendation on Infrastructure & Facility

Recommendation 3-1. The Department of Energy and the National Science Foundation should support the development of new instrumentation and techniques for the unique needs at the interface of chemistry and quantum information science. Broader access to laboratory-scale and mid-scale instrumentation is needed for the field to progress. For example, investments should be made in time-resolved magnetic resonance and optical spectroscopy. Support is required for professional staff to train users in the operation and utilization of these instruments, as well as to address new technique development and maintenance needs.