



NATIONAL SCIENCE FOUNDATION
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NSF 18-051

Dear Colleague Letter: Enabling Quantum Leap in Chemistry (QLC)

March 8, 2018

Dear Colleagues:

NSF recently unveiled 10 Big Ideas — bold, long-term research and process ideas at the frontiers of science and engineering.¹ Among these ideas, Quantum Leap aims to exploit quantum mechanical phenomena such as superposition and entanglement to develop next-generation technologies for sensing, computing, modeling, and communication. In the Fall of 2016, the Division of Chemistry (CHE) sponsored a workshop entitled "[Quantum Information and Computation for Chemistry](#)",² led by Alán Aspuru-Guzik of Harvard University and Michael Wasielewski of Northwestern University to explore the relevance of Quantum Leap to the field of chemistry. The workshop identified areas where chemists can contribute to Quantum Leap and areas where advances in Quantum Leap can enable the solution of intractable chemical problems. To follow up on the recommendations of the workshop, the CHE invites submission of [supplemental funding requests](#) and [EAGER \(EARly-Concept Grants for Exploratory Research\)](#) (EAGER) proposals on Quantum Leap.

This Dear Colleague Letter (DCL) emphasizes molecular approaches towards problems in quantum computing, sensing, communicating, etc. Suitable topic areas to address in EAGER proposals and supplemental funding request include (but are not limited to):

- quantum algorithms for the simulation of chemical systems, including hybrid quantum-classical algorithms;
- identification and exploration of the boundaries between classical and quantum computation in relation to chemical applications;
- quantum machine learning for chemistry;
- quantum optical tools for chemistry;
- bottom-up design, synthesis, and application of chemical qubits;
- quantum control of chemical processes;
- advanced quantum readout techniques for molecular quantum systems;
- topologically-protected molecular excitations that control and probe molecular energy transfer pathways via strong-coupling;

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- control and monitoring of chemical reactions using optical cavities and single-molecule polaritons; and
- multidimensional optical spectroscopy for quantum information processing.

Proposals or supplemental funding requests with a focus on solid state materials are outside the scope of this DCL.

The most competitive proposals and supplemental funding requests will harness existing expertise in the chemistry community to explore innovative approaches and novel phenomena in order to break new ground in quantum chemical and molecular science. These proposals and supplemental funding requests will also contain convincing evidence of the Principal Investigator's (PI's) competence in the proposed area of research and a clear path to future competitive research projects in Quantum Leap. Collaboration with experts in industry, national laboratories, and/or international researchers is encouraged, but not required.

Supplemental funding requests must enhance existing projects by incorporating or exploring the concepts described in this DCL. The upper limit of a supplemental funding request in response to this DCL is \$80,000 for a maximum of twelve months. EAGER proposals are limited to the funding amount and duration specified in the [NSF Proposal and Award Policies and Procedures Guide](#). They should be submitted to the CHE research program that is most closely aligned with the subject matter of the proposal.³

In all cases, Principal Investigators are strongly encouraged to contact the cognizant program officers⁴ prior to submission to determine the appropriateness of the work for consideration by sending email to QLChem@nsf.gov. For EAGER proposals, the title of the proposal should specify the title as: "QLC: EAGER: (title)".

Supplemental funding requests and EAGER proposals must be submitted by **May 1, 2018, 5:00 pm, submitter's local time.**

We are excited by the opportunities in Quantum Leap and look forward to working with the chemistry community to advance next generation quantum science. For general questions about this DCL, email the cognizant Program Officers in CHE⁴ at QLChem@nsf.gov.

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2. <https://arxiv.org/ftp/arxiv/papers/1706/1706.05413.pdf>
3. CHE research programs: <https://www.nsf.gov/funding/programs.jsp?org=CHE>.
4. QLC cognizant Program Officers: Evelyn Goldfield, Tingyu Li, Colby Foss, and John Papanikolas: QLChem@nsf.gov