U.S. NATIONAL SCIENCE FOUNDATION
2415 EISENHOWER AVENUE
ALEXANDRIA, VIRGINIA 22314

NSF 24-134

Dear Colleague Letter: NSF-UKRI/EPSRC Lead Agency Opportunity on Understanding and Exploiting Quantum Information in Chemical Systems

September 24, 2024

Dear Colleagues:

The U.S. National Science Foundation (NSF) and UK Research and Innovation (UKRI) have a Memorandum of Understanding (MOU) on Research Cooperation. The NSF-UKRI MOU provides an overarching framework to encourage collaboration between U.S. and U.K. research communities and sets out the principles by which jointly supported activities might be developed. The MOU provides for a lead agency opportunity whereby a single collaborative proposal between U.S. and U.K. researchers may be submitted to either NSF or UKRI, as described in NSF 23-128 ("Dear Colleague Letter: U.S.-UK Research Collaboration under the NSF-UKRI/Engineering and Physical Sciences Research Council Lead Agency Opportunity").

Under this Lead Agency Opportunity umbrella and through this Dear Colleague Letter (DCL), the NSF Directorate for Mathematical and Physical Sciences Division of Chemistry (NSF/MPS/CHE) and UKRI's Engineering and Physical Sciences Research Council (UKRI/EPSRC) are pleased to announce a joint funding call focusing on Quantum Information in Chemical Systems. In FY 2025 (October 2024-September 2025), UKRI/EPSRC will serve as the lead agency for all proposals. It is expected that in subsequent years NSF and UKRI/EPSRC will alternate serving as lead agency.

The goal of this activity is to promote transatlantic collaborative research by reducing some of the barriers that researchers may encounter in collaborative work. The lead agency opportunity allows U.S. and U.K. researchers to submit a single proposal describing a project involving both U.S. and U.K. groups. The proposal will undergo a single merit review process by the lead agency, on behalf of both NSF/MPS/CHE and UKRI/EPSRC. Proposers must provide a clear rationale for the need for a U.S.-U.K. collaboration, including a description of the unique expertise and synergy that the collaborating groups will bring to the project.

Proposals should be submitted to the funding call issued by UKRI/EPSRC (UKRI Funding Opportunity). They will be reviewed by UKRI/EPSRC and funding recommendations will be based on both success in merit review and the availability of funds from NSF/MPS/CHE and UKRI/EPSRC.

Proposals relevant to the following research area and agency programs are eligible for submission under this lead agency opportunity in FY 2025.

QUANTUM INFORMATION SCIENCE (QIS) IN CHEMISTRY

The fundamental understanding and the application of QIS concepts represents a significant scientific challenge for the chemistry community. Meeting this challenge will necessitate that the community draw upon its collective expertise in synthesis, measurement, and theory. With chemistry's nearly infinite ability in molecular design, there is the potential to design novel molecular systems that manifest desired quantum behavior for use in quantum computing, quantum sensing, and quantum communications. To this end, NSF/MPS/CHE and UKRI/EPSRC aim to strengthen the research on QIS in the context of chemical systems by fostering collaborations and synergies between research teams in the U.K. and in the U.S. The scope of this opportunity, which follows a bilateral workshop (https://arxiv.org/abs/2409.04264) hosted in Alexandria, Virginia, in February 2024, is for U.S. – U.K. collaborative research proposals that advance our fundamental understanding of QIS concepts in the context of chemical systems, or that leverage QIS concepts to advance chemistry research.

Research topics include but are not limited to these examples:

- Developing new ways of creating, observing, and quantifying QIS phenomena (e.g., quantum correlations, coherence, entanglement) in electronic, vibrational, and/or rotational quantum states of molecular systems.
- Studying the role of QIS phenomena (e.g., quantum correlations, coherence, entanglement) in chemical reactions, or exploiting those phenomena in the exploration of new reaction pathways.
- Developing new quantum sensors that can enhance our ability to monitor chemical systems and understand mechanisms.
- Developing new approaches that exploit quantum phenomena to visualize chemical systems at very short length scales and/or very fast time scales.

Proposals that include close, synergistic experimental and theoretical components are encouraged.

PROPOSAL PREPARATION AND SUBMISSION

In FY 2025, proposals in response to this lead agency agreement should be submitted to the

funding call issued by UKRI/EPSRC (UKRI Funding Opportunity). Proposers should submit one proposal only to UKRI/EPSRC. Proposers should follow the 2-stage application process described in NSF 23-128.

Please see the funding call issued by UKRI for proposal submission instructions and estimated timelines. Further information about due dates for full proposal submission will be communicated to applicants in the invitation from UKRI/EPSRC to submit full proposals. Only applicants who have submitted a qualified Expression of Interest (EOI) will be invited for full proposal submission.

Special instructions associated with submission of NSF-UKRI/EPSRC QIS Chemistry proposals:

1. Proposals that are inappropriate for funding by NSF/MPS/CHE or UKRI/EPSRC or are not responsive to this funding opportunity will not be invited for full submission or be returned without review, including but not limited to materials- or engineering-focused projects that are more appropriate for programs in the NSF Division of Materials Research or Engineering Directorate.
2. The US investigators must be eligible to submit proposals to NSF under the general guidelines contained in the *NSF Proposal & Award Policies & Procedures Guide* (PAPPG).
3. The proposal title should be prefaced with “UKRI-NSF:” to signify that UKRI is the lead agency.

MERIT REVIEW & AWARDS

In addition to the peer review, funding decision, and post-award considerations outlined in NSF 23-128, the following also apply:

1. Proposals submitted in FY25 will be reviewed in competition with other proposals received in response to the funding call issued by UKRI/EPSRC (UKRI Funding Opportunity).
2. Proposals will be reviewed in accordance with the lead agency's review criteria, in this case UKRI/EPSRC's. A description of the UKRI/EPSRC assessment process is available on the UKRI/EPSRC merit review website with additional details provided in the call issued by UKRI/EPSRC (UKRI Funding Opportunity) for this lead agency opportunity.
3. The lead agency may share proposal documents and reviews with the non-lead agency via secure file transfer, according to the lead agency’s confidentiality regulations. Only unattributed reviews and panel summaries will be shared between NSF/MPS/CHE and UKRI/EPSRC.
4. If a proposal is recommended for funding, the U.S. organization(s) will be supported by

NSF/MPS/CHE, and the U.K. organization(s) will be supported by UKRI/EPSRC. NSF/MPS/CHE and UKRI/EPSRC staff will review budgets to ensure that there are no overlaps or duplications in funding. Overlaps or duplications may lead to reduced funding or no award at all.

TIMELINE

EOI applications with UKRI/EPSRC will be evaluated on a rolling basis with the submission window closing in late November 2024. Invitations to submit full proposals will be made no later than early December 2024. The deadline for full proposal submission is expected to be in February 2025.

Proposers should consult the UKRI/EPSRC funding call (UKRI Funding Opportunity) for the exact deadlines for EOI and full proposal submission.

CONTACTS

UKRI/EPSRC Contacts

General questions should be directed to:

- International@epsrc.ukri.org

Specific programmatic inquiries should be directed to:

- Daniel Smith, Daniel.Smith@epsrc.ukri.org
- Sandra Lee, Sandra.Lee@epsrc.ukri.org

NSF/MPS/CHE Contacts

General questions should be directed to:

- che-epsrc@nsf.gov

Specific programmatic inquiries should be directed to:

- John Papanikolas, jpapanik@nsf.gov
- Richard Dawes, rdawes@nsf.gov
- Tingyu Li, tli@nsf.gov
- Colby Foss, cfoss@nsf.gov

Sincerely,

David Berkowitz, Assistant Director

Directorate for Mathematical and Physical Sciences