

**U.S. DEPARTMENT OF ENERGY  
OFFICE OF ENERGY EFFICIENCY AND RENEWABLE ENERGY  
NEPA DETERMINATION**



**RECIPIENT:** University of California, Riverside

**STATE:** CA

**PROJECT TITLE :** Large-Scale Density Functional Tight Binding (DFTB) Calculations to Probe Structural Effects and Bridge Multiple Length Scales in Hydrogen-Metal Systems

<b>Funding Opportunity Announcement Number</b>	<b>Procurement Instrument Number</b>	<b>NEPA Control Number</b>	<b>CID Number</b>
DE-FOA-0002598	DE-EE0010433	GFO-0010433-001	GO10433

**Based on my review of the information concerning the proposed action, as NEPA Compliance Officer (authorized under DOE Policy 451.1), I have made the following determination:**

**CX, EA, EIS APPENDIX AND NUMBER:**

Description:

<b>A9 Information gathering, analysis, and dissemination</b>	Information gathering (including, but not limited to, literature surveys, inventories, site visits, and audits), data analysis (including, but not limited to, computer modeling), document preparation (including, but not limited to, conceptual design, feasibility studies, and analytical energy supply and demand studies), and information dissemination (including, but not limited to, document publication and distribution, and classroom training and informational programs), but not including site characterization or environmental monitoring. (See also B3.1 of appendix B to this subpart.)
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Rationale for determination:

The U.S. Department of Energy (DOE) is proposing to provide funding to the University of California, Riverside (UCR) to evaluate failure mechanisms, predict thermodynamics/kinetics, and bridge multiple length scales to explore effects in hydrogen-metal systems when density functional theory (DFT) and large-scale density functional tight binding (DFTB) approaches are combined.

Award activities would explore the interplay between kinetics and hydrogen effects at cryogenic conditions, mechanisms of hydrogen-induced structural damage accumulation, and elucidating fundamental thermodynamic and kinetic behavior of these interactions. Findings would allow the Hydrogen Materials Compatibility Consortium (H-Mat) to augment their existing quantum and classical molecular dynamics capabilities.

Project activities would consist of desktop activities, literature searches, routine research, computer modeling, calculations, and writing within existing, purpose-built facilities. No change in the use, mission, or operation of existing facilities and locations would arise out of this effort. DOE does not anticipate any impacts to resources of concern due to the proposed activities of the project.

**NEPA PROVISION**

DOE has made a final NEPA determination.

Notes:

Hydrogen Fuel Cell Technology Office (HFTO)  
NEPA review completed by Amy Lukens, 4/3/2023.

**FOR CATEGORICAL EXCLUSION DETERMINATIONS**

The proposed action (or the part of the proposal defined in the Rationale above) fits within a class of actions that is listed in Appendix A or B to 10 CFR Part 1021, Subpart D. To fit within the classes of actions listed in 10 CFR Part 1021, Subpart D, Appendix B, a proposal must be one that would not: (1) threaten a violation of applicable statutory, regulatory, or permit requirements for environment, safety, and health, or similar requirements of DOE or Executive Orders; (2) require siting and construction or major expansion of waste storage, disposal, recovery, or treatment facilities (including incinerators), but the proposal may include categorically excluded waste storage, disposal, recovery, or treatment actions or facilities; (3) disturb hazardous substances, pollutants, contaminants, or CERCLA-excluded petroleum and natural gas products that preexist in the environment such that there would be uncontrolled or unpermitted releases; (4) have the potential to cause significant impacts on environmentally sensitive resources, including, but not limited to, those listed in paragraph B(4) of 10 CFR Part 1021, Subpart D, Appendix B; (5)

involve genetically engineered organisms, synthetic biology, governmentally designated noxious weeds, or invasive species, unless the proposed activity would be contained or confined in a manner designed and operated to prevent unauthorized release into the environment and conducted in accordance with applicable requirements, such as those listed in paragraph B(5) of 10 CFR Part 1021, Subpart D, Appendix B.

There are no extraordinary circumstances related to the proposed action that may affect the significance of the environmental effects of the proposal.

The proposed action has not been segmented to meet the definition of a categorical exclusion. This proposal is not connected to other actions with potentially significant impacts (40 CFR 1508.25(a)(1)), is not related to other actions with individually insignificant but cumulatively significant impacts (40 CFR 1508.27(b)(7)), and is not precluded by 40 CFR 1506.1 or 10 CFR 1021.211 concerning limitations on actions during preparation of an environmental impact statement.

The proposed action is categorically excluded from further NEPA review.

**SIGNATURE OF THIS MEMORANDUM CONSTITUTES A RECORD OF THIS DECISION.**

NEPA Compliance Officer Signature: \_\_\_\_\_



Electronically Signed By: Casey Strickland

NEPA Compliance Officer

Date: 4/4/2023

**FIELD OFFICE MANAGER DETERMINATION**

- Field Office Manager review not required
- Field Office Manager review required

**BASED ON MY REVIEW I CONCUR WITH THE DETERMINATION OF THE NCO :**

Field Office Manager's Signature: \_\_\_\_\_

Field Office Manager

Date: \_\_\_\_\_