

PMC-ND

(1.08.09.13)

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

**RECIPIENT:** Alex Zunger/University of Colorado Boulder**STATE:** CO

**PROJECT TITLE:** Accelerated Selection of Optimal Perovskite Alloys for Solar PV using a Combined Quantum and Machine Learning Hierarchical Approach

<b>Funding Opportunity Announcement Number</b>	<b>Procurement Instrument Number</b>	<b>NEPA Control Number</b>	<b>CID Number</b>
DE-FOA-0002357	DE-EE0009515	GFO-0009515-001	GO9515

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:

**A9 Information gathering, analysis, and dissemination** 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.)

**B3.6 Small-scale research and development, laboratory operations, and pilot projects** Siting, construction, modification, operation, and decommissioning of facilities for smallscale research and development projects; conventional laboratory operations (such as preparation of chemical standards and sample analysis); and small-scale pilot projects (generally less than 2 years) frequently conducted to verify a concept before demonstration actions, provided that construction or modification would be within or contiguous to a previously disturbed or developed area (where active utilities and currently used roads are readily accessible). Not included in this category are demonstration actions, meaning actions that are undertaken at a scale to show whether a technology would be viable on a larger scale and suitable for commercial deployment.

Rationale for determination:

The U.S. Department of Energy (DOE) is proposing to provide funding to University of Colorado Boulder (UCB) to develop a process for alloy identification/characterization utilizing quantum mechanics and machine learning algorithms. UCB would apply the machine learning algorithms developed as part of the project to screen alloy materials for solar cell applications. The materials would be further characterized in laboratory settings. The project would be completed over two Budget Periods (BPs), with a Go/No-Go Decision Point in between each BP. This NEPA Determination is applicable to both BPs.

Proposed project activities would consist of data analysis, algorithm development, material screening/characterization, material synthesis, and stakeholder engagement. Material characterization and synthesis would occur at laboratory scales (i.e., gram scales for solid input materials and liter scales for liquid input materials). Material synthesis would consist of the fabrication of perovskite-based thin film samples.

All project work would be coordinated by UCB. Data analysis, algorithm development, and material screening activities would be performed by UCB and its project partner University of South Carolina at research laboratories at their campuses in Boulder, CO and Columbia, SC, respectively. Material synthesis and characterization activities would be performed at the laboratory facilities of the National Renewable Energy Laboratory in Golden, CO. No physical modifications to existing facilities, ground disturbance, or changes to the use, mission, or operation of existing facilities would be required. No additional permits or authorizations would be required.

Project work would involve the use and handling of industrial chemicals, solvents, and potentially hazardous compounds (e.g., lead containing compounds). Nano-scale materials would also be utilized. All such handling would be performed in controlled laboratory environments that regularly conduct applied chemistry as part of their regular course of business. To mitigate potential hazards, UCB and its project partners would adhere to established institutional health and safety policies and procedures. Material synthesis and characterization, including all processes involving nano-scale materials, would be performed inside of a glovebox or fume-hood, where applicable.

Materials would be stored and transported in accordance with standard laboratory operating procedures. UCB and its project partners would observe all applicable Federal, state, and local health, safety, and environmental regulations.

Any work proposed to be conducted at a federal facility may be subject to additional NEPA review by the cognizant federal official and must meet the applicable health and safety requirements of the facility.

## NEPA PROVISION

DOE has made a final NEPA determination.

Notes:

Solar Energy Technologies Office

This NEPA determination does not require a tailored NEPA Provision.

NEPA review completed by Jonathan Hartman, 06/04/2021

## 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: Kristin Kerwin

NEPA Compliance Officer

Date: 6/4/2021

## 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: \_\_\_\_\_