ATTACHMENT B

STEWARDSHIP SCIENCE ACADEMIC ALLIANCES (SSAA)
FEDERAL ASSISTANCE APPLICATION FOR FOA DE-FOA-0002149
PROJECT SUMMARY INFORMATION SHEET

APPLICANT:

NAME Board of Trustees of the University of Illinois

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PRINCIPAL INVESTIGATOR:

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TYPE OF PROPOSED AWARD:
New Award

TOPICAL RESEARCH AREA:
Properties of Materials Under Extreme Conditions

PROJECT TITLE: Chicago/DOE Alliance Center – A Center of Excellence for High Pressure Science and Technology

OBJECTIVES: The goals of the Chicago/DOE Alliance Center (CDAC) are to significantly enhance our understanding of a broad range of materials in extreme pressure-temperature (*P-T*) regimes; to integrate and coordinate static compression, dynamic compression, and theoretical studies of materials; and to train the next generation of scientists for work in this field by enriching graduate education and training and by facilitating interactions between NNSA laboratory scientists and academia.

PROJECT DESCRIPTION: CDAC is dedicated to basic research, training, and technique development in the study of materials in extreme conditions. The Center has enabled numerous advances in high *P-T* science, technology, and training since its inception 16 years ago as the Carnegie/DOE Alliance Center. These advances include student and postdoc-led scientific discoveries and a successful track record in training early career scientists for work in the NNSA complex.

Materials of interest encompass crystalline solids, fluids and glasses, nanostructured to mesostructured materials, and complex composites. Chemically these materials include *d*- and *f*-electron elements and alloys, low-Z molecular compounds, energetic materials, dense gases, metal oxides and hydrides, and chemically heterogeneous substances. CDAC will advance understanding of these stewardship-related classes of materials in extreme conditions in the following six material property areas (1) *High P-T Structures and Phase Relations;* (2) *P-V-T Equations of State;* (3) *Phonons, Vibrational Thermodynamics, and Elasticity;* (4) *Plasticity, Yield Strength, and Deformation;* (5) *Electronic and Magnetic Structure and Dynamics; and* (6) *High P-T Chemistry*. CDAC will undertake selected research thrusts involving the above materials and property areas in the context of the following overarching grand challenges for extreme conditions science:

- *How can we understand, predict, and control matter and materials to very high compressions?*
- *What new physics may emerge in 'cold' to 'warm' dense matter?*
- *How can we accurately determine fundamental thermodynamic properties to high P-T multimegabars?*
- *How do defects, grain boundaries, and interfaces respond to high P-T conditions and strain rates?*
- *How can we better measure time-dependent transformations, and bridge strain-rate gaps between static, quasi-static, and dynamic compression?*
- *Can we better determine strength, plasticity, and rheology at ultrahigh P-T conditions?*
- *Can we expand the high P-T synthetic chemistry frontier to produce new, optimized materials?*

CDAC will conduct both static and dynamic compression experiments together with theory, modeling, and simulation in CDAC university laboratories as well as DOE/SC and DOE/NNSA facilities. The work will be enabled by continued access to CDAC's partner synchrotron radiation facilities, High Pressure Collaborative Access Team (HPCAT) at the Advanced Photon Source, Argonne National Laboratory (ANL) and the Frontier Infrared Spectroscopy (FIS) beamline at the National Synchrotron Light Source II, Brookhaven National Laboratory (BNL), as well as other facilities. The overarching scientific outcome is advancing fundamental understanding of materials behavior in extreme conditions, which in turn will lead to improved understanding of materials aging, performance of newly manufactured materials, materials in multiple extreme environments, and the creation of new materials.

CDAC engagement with NNSA programs at ANL and with its partner groups in Illinois will be significantly enhanced by its move to the University of Illinois at Chicago (UIC). CDAC will continue its active program in education and training of next-generation researchers for stewardship science. In so doing, CDAC will host student workshops and sponsor meetings and symposia for the broader community. The Center will facilitate student engagement with NNSA laboratories and be a vehicle for introducing early career scientists to NNSA laboratory programs. The Center will continue to closely collaborate with other academic groups, other SSAA awardees, and other national laboratory scientists. CDAC will continue to leverage the SSAA cooperative agreement with additional grants, which so far have multiplied by several times the impact and investment of NNSA in the Center. Finally, CDAC will continue to support use of NNSA facilities, including NIF, Z, and LANSCE, and feasibility studies for next-generation NNSA facilities. As such, CDAC will raise the visibility of the NNSA in the broader community.

CDAC will continue to be managed by Russell Hemley (Director) and Stephen Gramsch (Deputy Director) at UIC. Additional CDAC staff at UIC includes Muhtar Ahart, Ravhi Kumar, and Zhenxian Liu. Complementing this group are external Academic Partners Susannah Dorfman (Michigan State University), Elif Ertekin (University of Illinois at Urbana-Champaign) Steven Jacobsen (Northwestern University), Maik Lang (University of Tennessee), Lowell Miyagi (University of Utah) and Eva Zurek (University at Buffalo). Oversight and internal reviews of the program will continue to be provided by a Center Scientific Advisory Committee (CSAC) and an External Steering Committee (ESC).

MILESTONES: The principal *Outreach and Training* milestones include supporting every year 12 graduate students, 6 summer interns, an annual meeting, and a student workshop, and facilitating two CDAC student summer internship at the NNSA laboratories. The *Science* and *Technique Development* milestones are detailed in the Project Narrative and include completion of projects by CDAC students in the following range of topics: **Year 1:** Extreme states of water, including nucleation; pressurized doped UO_2; synchrotron studies of dense hydrogen and hydrides; non-equilibrium molecular dynamics; new electrical resistivity methods; ultrafast compression texture analysis. **Year 2:** microstructure evolution under extreme loads; x-ray and neutron scattering of superconductors and magnets; heterogeneous nucleation at high *P-T* solid-liquid interfaces; first-principles molecular dynamics simulations. **Year 3:** Strength and EOS at megabar stresses; doped and non-stoichiometric UO_2; heterogeneous nucleation in dynamic compression; superconductivity of *d*- and *f*-electron elements; deformation and texture development; mechanical response under extreme dynamic loads; modeling solid-solid phase transitions. **Year 4:** static and dynamic loading in heterogeneous materials; multiscale microstructure evolution; radiation tolerance of actinide compounds; non-equilibrium phase transitions; high *P-T* EOS of light element systems; stress-strain partitioning; local defect structures; combined high pressure and magnetic fields; mesoscale modeling for code validation.