Alexandra Navrotsky Institute for Experimental Thermodynamics (*AlexInstitute*)

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I. General Information, Designation and Benefit

*Name and Rationale for the Institute*

The proposed interdisciplinary administrative unit - *Alexandra Navrotsky Institute for Experimental Thermodynamics (*AlexInstitute*)* will serve as an aegis for experimental thermodynamics, focused on research that develops and employs modern calorimetric tools to advance scholarship in chemical engineering, chemistry, materials science, geochemistry, and related disciplines. As such, the *AlexInstitute* will enhance the careers of aspiring scientists, foster strong beneficial interactions among experimental thermodynamics researchers at WSU and with other experimental thermodynamics groups in the U.S. and worldwide, including those at the Pacific Northwest National Laboratory (PNNL). Although the work supported in the *AlexInstitute* will be limited to experimental thermodynamics as enabled by calorimetry, member faculty will also interact with individuals from other related fields, including computational and high pressure research. Thus the increased effort and future success are expected to benefit all such related efforts at WSU and elsewhere. The *AlexInstitute* is expected to participate strongly in large multidisciplinary and multi-institutional research proposals.

This *AlexInstitute* is enabled by Dr. Alexandra Navrotsky, who has recently established an endowment in the Voiland School of Chemical Engineering and Bioengineering (VSCEB) at Washington State University (WSU). Dr. Alexandra Navrotsky has provided a $1,000,000 gift to WSU. This fund is managed by the WSU Foundation and generates a spendable account, which will be managed by the VSCEB. Using WSU institutional policy, this gift should generate approximately $40,000 per year expendable funds to support the goals of the *AlexInstitute*. These funds are sufficient to support the goals of the *AlexInstitute*.

Fundamental thermodynamic data are of paramount importance in many current technologies, and play an ever-increasingly vital role in the foreseeable future. Thermodynamics of molecule – material interactions enforces the boundary conditions on many interfacial phenomena that govern the reactivity, selectivity, transformation and transportation of natural and engineered processes, while the energetic stability of materials dictates their synthesis, fabrication, utilization, storage, and disposition and/or recycle. Thus, it is necessary to understand the underlying thermodynamics of complex bulk and interfacial phenomena, especially as related to new materials and processes. By doing so, one can better tailor the synthesis of appropriate materials and understand the energetics of reactions to maximize the production of desired products and avoid undesired products, to minimize the
degradation of such materials in use, and to engineering robust waste forms once they retire. Such measurements are enabled by modern calorimetry, which measure the energy of atomic and/or molecular interactions between fluids and surfaces, the energy of molecular-level chemical reactions, including the formation and transformation of various solids. In the environmental and geochemical realm, calorimetry provides basic understanding of the fate and transport of nutrients and pollutants in water and soil, the availability and extraction of natural resources including minerals and oil, and the transformation and evolution, at present and in the distant past, on the surface and at great depth, on our planet and beyond it, of minerals, rocks, fluids, and melts.

The AlexInstitute will promote interdisciplinary experimental thermodynamics (calorimetric) research and will enhance the careers of aspiring scientists, especially women, specialized in experimental thermodynamics and calorimetry. Technically, the AlexInstitute will focus on the thermodynamics and energy landscapes of solid state materials, nanoparticles, clusters, and porous materials tightly related to energy harvesting and conversion, environmental remediation, and medicine. Its collaborative, innovative and transformative research will bridge fundamental research and technical applications, and benefit our society by providing thermochemical data and insight to engineers, materials scientists, earth and planetary scientists, and environmental scientists to understand complex systems and to use these systems to benefit society.

II. Infrastructure

Mission, Purpose and Goals

The mission of the AlexInstitute is to promote the fundamental, innovative, cutting-edge, interdisciplinary experimental thermodynamic (calorimetric) research that will lead to better understanding of the stability of materials and the interactions between atomic and/or molecular species and material surfaces that underscore solutions to global scale energy and environmental issues facing our civilization.

The general purpose of the AlexInstitute is to harness the power of experimental thermodynamics to address fundamental problems in chemical processes, such as catalysis, separations, materials synthesis, characterization, performance, and degradation, battery materials and the nuclear fuel cycle, seeking commonalities across a variety of phenomena and application in both technological and natural systems.

Through its transformative experimental thermodynamics research and scholarly activities, the AlexInstitute will achieve three major strategic goals in promoting interdisciplinary research:

1. Promote cutting-edge collaborative research leading to multi-PI and/or multi-institutional grants that are focused on critical energy, environmental, geological and medical issues. Examples include Department of Energy “Energy Frontier Research Centers” (DOE EFRC), and National Science Foundation “Science and Technology Centers” (NSF STC).

2. Lead outstanding experimental thermodynamic (calorimetric) research, including fundamental chemical and material studies as well as instrumental and technological development. The AlexInstitute aims at earning a reputation for world-class experimental thermodynamics research in five years.
3. According to the *Gift Use Agreement*, the *AlexInstitute* will use the proceeds from the endowment to:

- To the extent permitted by law and consistent with WSU policies, provide supplemental funding to attract and/or retain outstanding Ph.D. program graduate students and/or postdoctoral scholars, with preference given to female students/scholars (who may be designated as an *Alexandra Navrotsky Scholar*).

- Provide matching funds needed for grants from federal (e.g. National Science Foundation, US Department of Energy, US Department of Defense) or private (e.g. M.J. Murdock Charitable Trust) organizations.

- Purchase and set up new calorimetric equipment needed to advance the goals of the Institute.

- Enable travel to present research results at national or international meetings.

- Support other expenses connected with the conduct of the research by *AlexInstitute*-associated faculty.

*Nature and Scope of Research*

It is anticipated that the calorimetric research carried out by *AlexInstitute* will foster strong beneficial interactions with other experimental thermodynamics groups in the U.S. and worldwide, including those at PNNL. It will also interact with other related fields, including computational and high pressure research. Although its funding is to be limited to experimental thermodynamics, the increased effort and future success are expected to benefit all such related efforts at WSU and elsewhere. The *AlexInstitute* is expected to participate strongly in large interdisciplinary and multi-institutional research proposals.

*Expected Outcomes*

1. Elevate awareness of the critical role of experimental thermodynamics (calorimetry) in many research fields and promote interdisciplinary collaborations.

2. Leverage *AlexInstitute* to enable the purchase and installation of calorimetric equipment to advance the calorimetric technology and methodology.

3. Attract and retain at least two outstanding female Ph.D. students per year who have above a 3.5 undergraduate GPA, already published manuscripts in prestigious/high impact journals as the first author, and/or have been actively recruited by other institutions, who choose to pursue their graduate education at WSU because of the excellent scientific opportunities in the *AlexInstitute* and/or designation as an *Alexandra Navrotsky Scholar*.

4. Attract a major sponsored program that provides at least $250,000/y for several years and that supports Ph.D. students and postdoctoral scholars in both Chemistry and Chemical Engineering.
5. Host experimental thermodynamic workshops and conferences at WSU to promote interdisciplinary research using calorimetry. Organize similar workshops and conferences at appropriate national meetings.

6. Provide travel funds for graduate students and postdoctoral scholars to national and international meetings to present experimental thermodynamics research. The meetings where these results are to be presented should reflect interdisciplinary topics.

Unit Review and Assessment Plan

The unit review and assessment will be carried out yearly, in which the director of AlexInstitute provides a written report to the advisory board detailing the scholarly activity, including publications and conference presentation, grant application, funding leverage, and plan for the next calendar year. The advisory board members review the report, assess the plan, and provide guidance and feedback to the AlexInstitute on how to advance the science, faculty career and global impact. A two-hour advisory board meeting (teleconference) will be scheduled bi-yearly for the review and assessment. Moreover, one advisory board member will be invited to visit the AlexInstitute each year for on-site assessment.

Advisory Board

The advisory board of the AlexInstitute will serve as a resource through which the promotion of interdisciplinary collaborative research, development of calorimetric technology, and application of interdisciplinary multi-institutional proposals are advanced and assessed.

It will be composed of, at least two professors from universities, at least two research scientists from national laboratories, and at least one scientist/engineer from industry. Appointment to the advisory board will be for a five-year term. AlexInstitute-associated faculty will nominate and comment on board members but the appointment will be made jointly by the Director of the VSCEB and the Chair of the Department of Chemistry, after consultation with the AlexInstitute-associated faculty members.

Duties of the advisory board members will include:

1. Provide guidance, feedback and perspective regarding the interdisciplinary and multi-institutional research deriving from the AlexInstitute.

2. Help ensure the success of the AlexInstitute through feedback and internal assessment regarding the scientific and technical portfolio of the AlexInstitute.

3. Evaluate the report from the director of the AlexInstitute, and perform the yearly assessment.

4. Advocate for the AlexInstitute to broaden its scientific impact.

5. Advocate for subsequent gifts from other donors.

We propose the following individuals to be the founding advisory board members for the AlexInstitute:
Lynn A. Boatner – Corporate Fellow, UT Battelle Distinguished Inventor, and Group Leader, Oak Ridge National Laboratory, United States – Solid State Materials: Ceramics, Glasses, Alloys and Single Crystals

Nicolas Dacheux – Professor, French Alternative Energies and Atomic Energy Commission (CEA), France and University of Montpelier – Nuclear Sciences

Rodney C. Ewing (member of NAE) – Frank Stanton Professor in Nuclear Security, Stanford University, United States – Nuclear Materials, and Geochemistry

Bruce C. Gates (member of NAE) – Distinguished Professor, University of California, Davis, United States – Catalysis and Surface Science

James N. Petersen (ex officio) – Professor and Director, Voiland School of Chemical Engineering and Bioengineering, Washington State University, United States

Kirk Peterson (ex officio) – Edward R. Meyer Distinguished Professor and Chair, Department of Chemistry, Washington State University, United States

Yushan Yan – Distinguished Engineering Professor and Associate Dean for Research and Entrepreneurship for the College of Engineering, University of Delaware, United States – Nanostructured Materials for Energy, Environment, and Electronics


Stacey I. Zones (member of NAE) – Research Fellow and Consulting Scientist, Chevron Energy and Technology, United States – Zeolite and Catalysis

Administration and Membership

Initially, Di Wu (VSCEB) will be appointed as the founding Director leading the scholarly activity, interdisciplinary collaborative grant application and workshop/conference organization at the AlexInstitute. Additionally, the Director will draft the annual report, organize the advisory board meeting, and propose to use the funds. During a five-year period the director will work to enable a sustainable strategy to increase the impact and reputation of AlexInstitute. Upon the conclusion of Di Wu’s five-year cycle, Director of the VSCEB and the Chair of Chemistry will consult with AlexInstitute-associated faculty and then appoint the Director. Directors may serve consecutive terms.

The fund of AlexInstitute will reside in VSCEB at WSU, and the management will follow institutional policies. The proceeds of fund will be used to advance the experimental thermodynamic (calorimetric) research conducted by the faculty participating in the Institute, as determined by the Director of the AlexInstitute, the Director of VSCEB, and Chair of the Department of Chemistry in consultation with the AlexInstitute faculty.

Initially, the key faculty members participating in the AlexInstitute will include Drs. Di Wu (VSCEB) and Xiaofeng Guo (Chemistry), whose research cover calorimetric studies on catalysis and surface phenomena (Wu), porous and composite materials development (Wu), materials for clean energy (Guo and Wu), and nuclear science (Guo and Wu). Additional
faculty may be invited to join the Institute, provided such faculty have active research programs centered in experimental thermodynamics (calorimetry) and are approved by > 80% AlexInstitute members.

To guarantee the leading role of the AlexInstitute in calorimetry and the quality of AlexInstitute-associated faculty. Specifically, the additional faculty invited must satisfy the following criteria:

1. The individual must hold an appointment as a WSU faculty member.
2. The individual’s primary research focus must be experimental thermodynamics (calorimetry).
3. The individual’s research must center on the design, advancement, and/or application of calorimetry technology or methodology.
4. The individual must be the PI or co-PI on at least one competitively awarded grant sufficient to support at least one full-time Ph.D. student for the duration of the grant for three consecutive years prior to appointment as a member.
5. The individual must be a highly active scholar in the field of experimental thermodynamics and calorimetry, serving as the corresponding author for at least 10 publications over the previous 5 years.
6. Members will be appointed for 5 year, renewable periods.

Financial Support and University Resources

There is no university financial support or resources needed for the current stage. It is anticipated that in the normal course of business, the various dean(s) may articulate hiring plans that include positions for faculty who conduct experimental thermodynamics research. If such positions are articulated by the appropriate dean(s), then the AlexInstitute could serve to help attract outstanding individuals to WSU. No hiring is requested as a part of this proposal to establish the AlexInstitute. Additionally, it is emphasized that the AlexInstitute is designed to help attract sponsored program funds to WSU, and no expectation for institutional investment is requested as the Institute is established. The VSCEB and the WSU Chemistry have provided appropriate research laboratories and offices for Drs. Wu and Guo. No additional support will be provided by the VSCEB and the WSU Chemistry for the AlexInstitute beyond those which would be provided to any faculty member in these departments.

University Endorsement

Letter from Director, Dean, and/or Provost (attached).