The energy industry is being digitally transformed by investment at all levels of production, generation, transmission, and distribution: sensors, data analytics, new privacy-aware markets, and usage of smart meters in homes are all part of this transformation. However, the transformation of energy to be resilient to large environmental changes, faults (including maintenance errors), and cyber-attacks is still a work in progress. The early lead of energy operators in embracing digital transformation has enabled those systems to use digital transformation not only to enhance energy efficiency but also to lead the way to a lower-carbon, higher-efficiency economy that will enhance both energy and climate security.

This C3DTI Second Call for Proposals addresses the challenges for AI and Digital Transformation for Energy and Climate Security.

Areas of interest include but are not restricted to:

1. **Sustainability**: Applying AI/ML and advanced analytic techniques to support sustainability initiatives. Areas of focus may include scalable and trustworthy techniques for energy consumption analysis, supply chain and Scope 3 energy and emissions analyses (see [EPA Scope 3 Inventory Guidance](https://www.epa.gov/energy/scope-3-inventory-guidance)).
2. **AI for Carbon Sequestration**: Applying AI/ML techniques to increase the scale and reduce the cost of carbon sequestration. Areas of focus may include AI for advanced materials research to build better extraction of carbon dioxide (CO2) from the atmosphere, petrochemical process optimization for carbon capture, fossil fuel decarbonization, site-specific modeling of geophysical sequestration and emissions containment, and new sequestration technologies.
3. **AI for Leaks and Emissions Detection**: Applying advanced AI/ML techniques for large scale emissions detection, facility-level data reconciliation and gap analysis for emissions sensors, prediction of emissions risk, and analysis and optimization of flaring intensity across upstream and downstream operations.
4. **Safe Hydrocarbon Production and Transportation Infrastructure**: Applying analytic and AI/ML modeling techniques to increase the safety and reduce emissions from oil and gas extraction, petrochemical production, and hydrocarbon transportation. Areas of focus may include AI-based and imaging algorithms to detect potential hazards and reduce accidents, with particular application in multi-modal sensing and drone-based real-time detection of methane and CO2 leaks, AI-based predictive maintenance, AI-enabled corrosion detection, AI-supported augmented reality systems for maintenance support, and next-generation AI-based digital twinning to support the modeling of hydrocarbon systems.
5. **AI for Advanced Energy and Carbon Markets**: Enabling dynamic, automated, and real-time pricing of energy generation sources. Areas of focus may include distributed resources, spinning reserve and voltage support, renewables, peer-to-peer energy transactions, improved energy and carbon price forecasting, and mechanism design to positively incentivize energy and carbon markets and prevent free riding and adverse selection.
6. **Cybersecurity of Power and Energy Infrastructure**: Leveraging AI/ML techniques to improve the cybersecurity of our critical power and energy assets, as well as smart connected factories and homes. Areas of focus may include AI/ML for distributed hardware and network management, detection of anomalous network activity and log monitoring, and the cohesive analysis of hybrid Information Technology (IT) and Operational Technology (OT) systems.
7. **Smart Grid Analytics**: Applying AI and other analytic approaches to improve the efficiency and effectiveness of grid transmission and distribution operations. Areas of focus may include Volt/VAR optimization, non-technical loss reduction, predictive maintenance for the grid, accelerated outage detection and recovery, automated power routing, grid management given load profiles of Electric Vehicles, and improved control and operation of microgrids.
8. **Distributed Energy Resource Management**: Applying AI to increase the penetration and use of distributed renewables. Areas of focus may include improving grid efficiency with renewables, granular load forecasting, automated demand-response, appropriate policy design, and the optimal dispatching of distributed resources.
9. **AI for Energy-Efficient Buildings and Factories**: Leveraging AI techniques for advanced building and factory control to improve energy efficiency. Areas of focus may include AI-based motor control systems, advanced load disaggregation analyses, direct load control, and optimal pre-cooling or heating to minimize costs and stress on energy networks.
10. **AI for Improved Natural Catastrophe Risk Assessment**: Applying AI to improve modeling of natural catastrophe risks from future weather-related events (e.g., tropical storms, wildfires, floods). Areas of focus may include advanced asset vulnerability models, the prioritization of climate adaptation measures to enable rapid and more effective disaster recovery, and the appropriate portfolio and pricing of risk transfer solutions.
11. **Resilient Energy Systems**: Addressing how the use of AI/ML techniques and markets for energy and carbon introduce new vulnerabilities. Areas of focus may include detecting cyber-attacks, including Advanced Persistent Threats (APTs), mitigating the risks from such attacks, and operating resiliently through such attacks.
12. **AI for Improved Climate Change Modeling**: Using AI/ML to address climate change modeling and adaptation. Areas of focus may include deep-learning based fine-scale cloud models to enhance larger-scale climate models, circulation models of the stratosphere and troposphere, multi-scale modeling of weather phenomena, processes that govern climate variability and change, and methods to predict climate variations, extended weather, and climate predictability.

All proposals should be submitted online via EasyChair at:

https://easychair.org/conferences/?conf=c3dticfp2

Proposals must be submitted to EasyChair by 11:59 pm PDT March 29, 2021.

Awards will be announced in late May 2021, with start dates of June 1, 2021.
C3DTI will host a series of online information sessions and to provide an overview of the call for proposals and discuss the computing resources available to Research Award recipients as well as office hours with technical staff. Below are the dates and times for each information session and details about office hours.

**General Information Sessions (Online)**

- **Monday, February 15, 11 am – 12 pm PT / 2 – 3 pm ET**
  Zoom Meeting: [https://berkeley.zoom.us/j/92742836523](https://berkeley.zoom.us/j/92742836523)

  - This online information session will provide an overview of the C3.ai DTI and the second call for proposals and provide an opportunity for proposers to ask questions or get clarification as they prepare proposals.

- **Wednesday, February 17, 11 am – 12 pm PT / 2 – 3 pm ET**
  Zoom Meeting: [https://berkeley.zoom.us/j/95629876415](https://berkeley.zoom.us/j/95629876415)

  - This online information session will provide an overview of the C3.ai DTI and the second call for proposals and provide an opportunity for proposers to ask questions or get clarification as they prepare proposals.

**Computing Resources Information Sessions (Online)**

- **Friday, February 19, 10 – 11 am PT / 1 – 2 pm ET**
  Zoom Webinar: [https://berkeley.zoom.us/j/96277461240](https://berkeley.zoom.us/j/96277461240)

  - This online information session will provide an overview of the C3 AI Suite and the available supporting resources.

- **Tuesday, February 23, 2 – 3 pm PT / 5 – 6 pm ET**
  Zoom Webinar: [https://berkeley.zoom.us/j/95880959454](https://berkeley.zoom.us/j/95880959454)

  - This online information session will take a deeper dive into the capabilities of the C3 AI Suite.

- **Tuesday, March 2, 10 – 11 am PT / 12 – 1 pm ET**
  Zoom Webinar: [https://berkeley.zoom.us/j/99845556376](https://berkeley.zoom.us/j/99845556376)

  - This online information session will discuss Ex Machina, a C3 AI tool that enables anyone to develop, scale, and apply AI insights without writing code.

**Weekly Office Hours (Online)**

Additionally, the C3DTI Development Operations and C3 AI technical support teams will be available every Tuesday from 2 – 3 pm PT / 5 – 6 pm ET between March 2 and March 23.

Zoom Meeting: [https://illinois.zoom.com.cn/j/87825348092?pwd=c1k1VWkxRXRQO0FzUnN0O256Zz09](https://illinois.zoom.com.cn/j/87825348092?pwd=c1k1VWkxRXRQO0FzUnN0O256Zz09)

Questions about general eligibility, proposal preparation, or research awards should be directed to the C3DTI by e-mail at proposals@c3dti.ai.

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**Colloquium on Digital Transformation Science**

Teresa Head-Gordon, Chancellor’s Professor, Department of Chemistry, Chemical and Biomolecular Engineering, and Bioengineering, University of California, Berkeley

REGISTER FOR ZOOM WEBINAR

The rapid spread of SARS-CoV-2 has spurred the scientific world into action for therapeutics to help minimize fatalities from COVID-19. Molecular modeling is combating the current global pandemic through the traditional process of drug discovery, but the slow turnaround time for identifying leads for antiviral drugs, analyzing structural effects of genetic variation in the evolving virus, and targeting relevant virus-host protein interactions is still a great limitation during an acute crisis. The first component of drug discovery - the structure of potential drugs and the target proteins - has driven functional insight into biology ever since Watson, Crick, Franklin, and Wilkins solved the structure of DNA. What could we do with structural models of host and virus proteins and small molecule therapeutics? We can further enrich structure with dynamics for discovery of new surface sites exposed by fluctuations to bind drugs and peptide therapeutics not revealed by a static structural model. These “cryptic” binding sites offer new leads in drug discovery but will only yield fruit if they can be assessed rapidly for binding affinity for new small molecule drugs. We offer physics-inspired data-driven models to: 1) extend the chemical space of new drugs beyond those available; 2) create reliable scoring functions to evaluate drug binding affinities to cryptic binding sites of COVID-19 targets; 3) accelerate computation of binding affinities by training machine learning models; and 4) closing the loop of design and evaluation to bias the distribution of new drug candidates towards desired metrics enabled by the C3 AI Suite.

Teresa Head-Gordon - The simultaneous revolutions in energy, molecular biology, nanotechnology, and advanced scientific computing is giving rise to new interdisciplinary research opportunities in theoretical and computational chemistry. The research interests of the Teresa Head-Gordon lab embraces this large scope of science drivers through the development of general computational models and methodologies applied to molecular liquids, macromolecular assemblies, protein biophysics, and homogeneous, heterogeneous catalysis and biocatalysis. She has a continued and abiding interest in the development and application of complex chemistry models, accelerated sampling methods, coarse graining, and multiscale techniques, analytical and semi-analytical solutions to the Poisson-Boltzmann Equation, and advanced self-consistent field (SCF) solvers and SCF-less methods for many-body physics. The methods and models developed in her lab are widely disseminated through many community software codes that scale on high performance computing platforms.