**NEXT GENERATION WORK**

Next generation Track-1 systems in the coming years will enable us to carry out more systematic analyses on a larger class of materials. Our initial work shows that simulations of larger sized systems are important. Also, more systematic studies will enable us to carry out big data assessments of correlated many-body wave functions, towards the idea of “correlated electron genomics.”

**COLLABORATIVE RESEARCH: INNOVATIVE AB INITIO SYMMETRY-ADAPTED NO-CORE SHELL MODEL FOR ADVANCING FUNDAMENTAL PHYSICS AND ASTROPHYSICS**


**INTRODUCTION**

One of the quintessential open challenges in contemporary physics is to design a comprehensive many-body theory for modeling and predicting nuclear structure and reactions starting from inter-nucleon forces that are consistent with the underlying theory of Quantum Chromodynamics (QCD). The ultimate goal of ab initio theory is to find a solution to this problem, which is a computationally-intensive endeavor due to a dual challenge, namely, the non-perturbative nature of QCD in the low-energy regime and the complexity of many-particle nuclei. Short-lived nuclei, currently inaccessible to experiment, are key to understanding processes in extreme environments. From stellar explosions to the interior of nuclear reactors, first-principle nuclear models that hold predictive capabilities have been and will be demonstrating a tremendous impact on advancing our knowledge at the frontiers of astrophysics, neutrino physics, and applied physics.

**METHODS & RESULTS**

We have developed an innovative ab initio nuclear structure approach, symmetry-adapted no-core shell model (SA-NCSM) [1], with concomitant computer code dubbed LSZNCSM II [2], that embraces the first-principles concept and capitalizes on a new symmetry of the nucleus. The ab initio SA-NCSM solves the time-independent Schrödinger equation as a Hamiltonian matrix eigenvalue problem. The main computational task is to evaluate a large symmetric Hamiltonian matrix and to obtain the lowest-lying eigenvectors that correspond to the experimental regime. Accuracy is based on the degree of convergence, which is linked to the size of the model space that can be achieved. The SA-NCSM utilizes physically relevant model space of significantly reduced dimensionality compared to ultra-large model spaces encountered by standard ab initio approaches. These theoretical advances coupled with the computational power of Blue Waters allow us to reach medium-mass nuclei that are inaccessible experimentally and fall far beyond the limits of other ab initio methods. The nuclei of interest represent a considerable challenge requiring immensely intensive endeavor due to a dual challenge, namely, the non-perturbative nature of QCD in the low-energy regime and the complexity of many-particle nuclei. Short-lived nuclei, currently inaccessible to experiment, are key to understanding processes in extreme environments. From stellar explosions to the interior of nuclear reactors, first-principle nuclear models that hold predictive capabilities have been and will be demonstrating a tremendous impact on advancing our knowledge at the frontiers of astrophysics, neutrino physics, and applied physics.

**PUBLICATIONS AND DATA SETS**

Allocations: NSF PRAC/100Mh
PI: J. P. Drayer
IU: Louisana State University
IU: Czech Academy of Sciences and Louisiana State University
IU: Iowa State University
IU: Ohio State University
IU: Old Dominion University
IU: Czech Technical University
IU: University of North Carolina
IU: Princeton University

**EXECUTIVE SUMMARY**

We use Blue Waters to carry out large-scale modeling of light and medium-mass nuclei, including short-lived nuclei not yet accessible to experiment but critical to understanding astrophysical processes, which are the focus of current and next-generation rare isotope experimental facilities. The scale of computational challenges inherent to modeling such intricate quantum many-body systems makes the utilization of Blue Waters resources essential for addressing long-lasting challenges of importance to nuclear theory and experiment, as well as astrophysics. Breakthrough theoretical advances [1] coupled with Blue Waters’ cutting-edge computational power have opened a new region, the intermediate-mass nuclei from fluorine (F) to calcium (Ca) isotopes, for first investigations with ab initio methods. This breakthrough fundamentally advances our understanding of nuclear synthesis, as nuclear energy spectra and reaction rates for many short-lived nuclei involved in nuclear synthesis are not yet accessible by experiment or reliably measured for the astrophysically relevant energy regime.

**WHAT BLUE WATERS**

Ab initio nuclear structure studies represent an extremely computing-intensive endeavor. To illustrate the level of complexity, applications to medium-mass nuclei require over hundreds of exabytes of memory to store the Hamiltonian description.
The major increase in computational power provided by the second generation of Track-I system, along with emergent algorithms designed to take advantage of modern massively parallel architectures, will enable ab initio theories to start providing information of unprecedented quality for probing fundamental symmetries and physics beyond the standard model. Furthermore, increased computational resources will allow the SA-NCSM framework to address even heavier nuclear systems. For example, addressing neutronless double beta decay for 46Ca should become feasible at a level that will reduce large uncertainties in the nuclear structure matrix elements and allows one to determine the neutron type from planned experiments, which represents one of the most fundamental problems in physics today.

**PUBLICATIONS AND DATA SETS**


**NEXT GENERATION WORK**

The major increase in computational power provided by the second generation of Track-I system, along with emergent algorithms designed to take advantage of modern massively parallel architectures, will enable ab initio theories to start providing information of unprecedented quality for probing fundamental symmetries and physics beyond the standard model. Furthermore, increased computational resources will allow the SA-NCSM framework to address even heavier nuclear systems. For example, addressing neutronless double beta decay for 46Ca should become feasible at a level that will reduce large uncertainties in the nuclear structure matrix elements and allows one to determine the neutron type from planned experiments, which represents one of the most fundamental problems in physics today.

**EXECUTIVE SUMMARY**

Silicon (Si) is one of the most promising electrode materials for high-performance lithium (Li) ion batteries because it has an order of magnitude higher specific capacity compared to conventional graphite electrodes. However, Si electrodes crack massively during Li insertion since they expand by 300% when fully-lithiated; they also delaminate from the current collector after many charge cycles. We have conducted large-scale parallel molecular dynamics simulations and density functional theory calculations on Blue Waters to uncover the underlying mechanisms for cracking and delamination of the Si electrode during charge cycling; these mechanisms are in excellent agreement with experiments. Blue Waters resources were needed because of the computational scale of the problem and the many computational runs needed to cover the entire parameter space. Our results have provided rich insights into the design and engineering of damage tolerant electrode materials for high-capacity Li-ion batteries.

**INTRODUCTION**

Lithium ion batteries are high-energy-dense systems that store energy by insertion of Li ions into solid electrodes. Silicon is one of the most promising electrode materials for high-performance Li-ion batteries since it possesses the highest known specific capacity of 4200 mAh/g, which is an order of magnitude greater than conventional graphite electrodes. During lithiation, the Si electrodes form Li$_x$Si compounds and undergo huge volume expansion of about 300% since one Si atom can theoretically bond with a maximum of x = 3.75 Li atoms. When attached to a metal current collector, such as copper (Cu), the massive and inhomogeneous

**NANOSCALE MECHANICS OF DEFORMATION IN HIGH-CAPACITY LITHIUM-ION BATTERIES**

Allocation: Illinois/291 Kish
PI: Hsueh Beng Chew

1University of Illinois at Urbana-Champaign

**FIGURE 2**: Density profile of the surprising intrinsic structure.