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RPPR Final Report

as of 14-Jan-2019

Agency Code:

Proposal Number: 66878CHRIP

Agreement Number: W911NF-15-1-0344

INVESTIGATOR(S):

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Report Date: 14-Nov-2016

Date Received: 09-Jan-2019

Final Report for Period Beginning 15-Aug-2015 and Ending 14-Aug-2016

Title: High Performance Beowulf Cluster for Computational Studies of Electrolytes for Energy Storage and Conversion

Begin Performance Period: 15-Aug-2015

End Performance Period: 14-Aug-2016

Report Term: 0-Other

Submitted By: Stephen Paddison

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Distribution Statement: 1-Approved for public release; distribution is unlimited.

STEM Degrees: 1

STEM Participants: 3

Major Goals: The purpose of this DURIP grant is to acquire a small Beowulf computational cluster consisting of eight compute nodes that will be integrated into the PI's existing computational cluster.

This state of the art cluster will permit electronic structure calculations to be performed on large molecular systems with highly accurate quantum chemical methodologies (e.g. MP2, G2, QCISD, etc.) that may be used to assess the short coming in DFT based methods). The cluster will also be utilized to perform trial and benchmarking AIMD simulations (e.g. with the VASP code) for the submission of proposals requested computational time on the large supercomputer centers across the country (i.e., via the XSEDE).

The calculations and simulations performed with this equipment will permit the ARO funded research on various polymerized ionic liquids (Proposal Number: 67802-CH, Agreement Number: W911NF-16-1-0402).

Accomplishments: A Beowulf computational cluster consisting of eight compute nodes each (node) featuring Intel Xeon Haswell motherboards and IVY Bridge 2.6 GHz processors with 25 MB of level cache was purchased. The nodes have 16 cores (each) with 256 GB and 12 TB of memory and disk storage space, giving the entire cluster slightly more than 256 GB and 12 TB of memory and storage, respectively. All the nodes are connected with a very low-latency high-bandwidth QDR Infiniband MPI network which has a latency of only a few microseconds and bandwidth of 40 Gb/s.

This cluster was integrated into the PI's existing (but much inferior) cluster and has served as the 'work horse' for the undertaking of very extensive electronic structure calculations with highly accurate (but computationally expensive) methodologies. The cluster has also served the purpose of running a number of trial and benchmarking ab initio molecular dynamics (AIMD) simulations and dissipative particle dynamics (DPD) simulations. These test and small system simulations have been critical in securing computational time and eventual results on the Texas Advanced Supercomputer Center (TACC). The PI and his group has utilized millions of CPU hours at the TACC to undertake simulations of the electrochemical systems and materials studied in the ARP funded research.

Furthermore, all of the analysis of the simulations have been performed on this computational cluster.

During the past 3 years this computer cluster has been critical in the research that has resulted in 8 publications.

Training Opportunities: One postdoctoral researcher and 3 Ph.D. students have all extensively utilized this Beowulf cluster. The students have all received training on DPD and AIMD simulation techniques.

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Results Dissemination: “Polymerized Ionic Liquids: Correlating Morphology with charge transport”, invited talk, ARO Chemical Sciences Division Program Review, sponsored by the Army Research Office, Durham, NC July 30th – August 1st, 2018.

“Structure/Function Relations in Ion Containing Polymers”, invited departmental seminar, Department of Chemistry, Technical University of Munich, Garching, Germany June 29th, 2018.

“Quantitative Structure Analysis of Polymerized Ionic Liquids with Atomistic Molecular Simulations”, invited talk, NAMS 2018 Annual Meeting, Membranes for Energy Applications (Storage Battery to Fuel Cells), Lexington, KY June 9th – 13th, 2018.

“Structure/Function Relations in Ion Containing Polymers”, invited departmental seminar, Department of Chemistry, University of Calgary, Calgary, Canada February 2nd, 2018.

“Quantifying Water Distribution and Connectivity in Ionomers: Comparison of Hydrated Nafion and Nafion/Polybenzimidazole Systems”, invited talk, Symposium I01C: Polymer Electrolyte Fuel Cells 17 (PEFC 17) – Cation-Exchange Membrane Performance and Durability, 232nd Meeting of the ECS, National Harbor, MD October 1st – 5th, 2017.

“Polymerized Ionic Liquids: MD Simulations & Experiments”, invited talk, ARO Chemical Sciences Division Program Review, sponsored by the Army Research Office, Archie K. Davis Conference Center, Research Triangle Park, Durham, NC August 7th – 11th, 2017.

“Coarse-grained simulations of PFSA/PBI membranes”, invited seminar, Institut Charles Gerhardt, Université Montpellier 2, Montpellier, France July 19th, 2017.

“Multiscale Modeling of Battery & Fuel Cell Electrolytes”, invited talk, Polymers for Fuel Cells, Energy Storage & Conversion, sponsored by Division of Polymer Chemistry, American Chemical Society, Pacific Grove, CA Feb. 26th – March 1st, 2017.

“Understanding the Morphology of Proton Conducting Composite Membranes through Simulation”, invited talk, Symposium: EC5: Proton Transfer and Transport—From Biological Systems to Energy Applications, Fall Meeting of the MRS, Boston, MA Nov. 27th – Dec. 2nd, 2016.

“Multiscale modelling of Soft Matter”, International School on Electrochemical Energy Conversion and Storage, MPI for Solid State Research, Stuttgart, Germany, October 24th – 26th, 2016.

“Morphology of Elastomeric Anion Exchange Membranes: A Dissipative Particle Dynamics Study”, PRIME meeting of the ECS, Hawaii Convention Center, Honolulu, HI October 2nd – 7th, 2016.

“Understanding the Morphology of Proton Conducting Composite Membranes through Simulation”, invited talk, Solid State Proton Conductors - 18, Soria Moria Conference Center, Oslo, Norway September 18th – 23rd, 2016.

“Vn+ in PFSA Membranes: Ab Initio and Classical Simulations”, CERM 2016, 47th Central Regional Meeting of the ACS, Molecular Modeling of Energy Storage Devices & Biomolecular Complexes, Covington, KY May 18th – 21st, 2016.

Honors and Awards: Nothing to Report

Protocol Activity Status:

Technology Transfer: Nothing to Report

PARTICIPANTS:

Participant Type: PD/PI

Participant: Stephen J Paddison

Person Months Worked: 12.00

Funding Support:

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Project Contribution:
International Collaboration:
International Travel:
National Academy Member: N
Other Collaborators:

Participant Type: Postdoctoral (scholar, fellow or other postdoctoral position)

Participant: Hongjun Liu

Person Months Worked: 12.00

Funding Support:

Project Contribution:
International Collaboration:
International Travel:
National Academy Member: N
Other Collaborators:

Participant Type: Graduate Student (research assistant)

Participant: Xubo Liu

Person Months Worked: 12.00

Funding Support:

Project Contribution:
International Collaboration:
International Travel:
National Academy Member: N
Other Collaborators:

Participant Type: Graduate Student (research assistant)

Participant: Zhenghao Zhu

Person Months Worked: 6.00

Funding Support:

Project Contribution:
International Collaboration:
International Travel:
National Academy Member: N
Other Collaborators:

Nothing to report.