Computational Design of New Materials for Energy and Environmental Applications

Karl Johnson, Department of Chemical & Petroleum Engineering

Resource Allocation Request

The following sections should be filled out in accordance with the CRC's Resource Allocation Request Guidelines: https://crc.pitt.edu/Pitt-CRC-Allocation-Proposal-Guidelines. Failure to do so will result in requests for revisions.

Resource Type	SUs Requested	Maximum SUs allowed
MPI	1,888,800	**3,200,000**
SMP standard (default)	1,242,720	**1,700,000**
HTC	0	**1,000,000**
GPU	53,300	**300,000**

The sum of the "SUs Requested" column should not be more than 3,200,000 SUs.

Project Abstract

Our CRC request is dependent on three funded projects. Project 1 is "Computational Design and Machine Learning-Assisted Search for Dual-Function MOFs towards Nerve Agent and Blistering Agent Detoxification". We are performing three types of calculations for this project: (1) quantum mechanical calculations of molecules and nanoporous materials; (2) classical empirical calculations for statistical mechanical molecular simulations; (3) large-scale machine learning calculations for development and application of ML potentials. Project 2 is "Energy Harvesting and Storage with Gradient Hybrid MOFs" and involves periodic and cluster quantum mechanical calculations. Project 3 is "FLOSIC: Efficient density functional calculations without self-interaction" and involves density functional theory and wavefunction calculations.

Justification of SU Amount Requested

MPI Partition

DFT calculations with VASP for systems having over 100 atoms will run efficiently in the MPI . The specific jobs are outlined below.

1. CI-NEB calculations require 5 nodes on MPI, each about 28800 SUs. We estimate 10 jobs, total of 288000 SUs
2. MD simulations for training DPs require 2 nodes, about 9200 SUs each and we project 150 such simulations for a total of 1380000 SUs
3. Single point calculations for DP active learning, 2 nodes, 9 hours each, estimated 20000 jobs for a total of 180000 SUs
4. Ionic relaxations require about 1700 SUs per job and we estimate 24 such jobs for a total of 40800 SUs

Total MPI SUs = 1,888,800

SMP Partition

The types of jobs here include VASP with a smaller number of atoms, ORCA, Gaussian, LAMMPS, and RASPA. There are a host of different types of jobs. We estimate a total need of 1,242,720 SUs.

Job description	Cluster	Nodes	Cores	SUs/job	# of jobs	SUs total
Diffusion of fluids in defective MOFs	SMP	1	64	9216	100	921600
RASPA adsorption isotherms	SMP	1	1	144	240	34560
CCSD(T) sp of small clusters	SMP	1	24	1728	40	69120
DFT optimizations of small clusters	SMP	1	24	576	40	23040
FLO-SIC calculations	SMP	1	24	720	170	122400
MOF linker optimizations	SMP	1	12	1152	40	46080
Linker IR/Raman	SMP	1	12	576	40	23040
TDDFT calculations	SMP	1	12	72	40	2880
					Total SMP:	**1242720**

GPU Partition

We will use the GPU partition for training and production runs of our Deep-learning Potentials (machine learning with DeePMD)

We estimate a total of 53,600 SUs

DP training	GPU	1	1	12	300	3600
Model deviation	GPU	1	1	1	20000	20000
DP Production	GPU	1	1	60	500	30000
					Total GPU:	**53600**

Additional Information

Funding Sources for projects using CRC Resources:

PI:	J. K. Johnson; Co-PI: L. L. Huang (University of Oklahoma)
Agency:	DTRA
Grant No.:	HDTRA12410009
Amount:	$200,000
Location:	University of Pittsburgh
Duration:	03/11/24 – 03/10/25
Effort:	0.45 calendar months
Title:	Computational Design and Machine Learning-Assisted Search for Dual-Function MOFs towards Nerve Agent and Blistering Agent Detoxification

PI:	J. K. Johnson; Co-PIs: J. Millstone (Pitt), N. L. Rosi (Pitt), R. Frontiera (U. Minnesota), E. Borguet (Temple U.)
Agency:	DTRA
Amount:	$2,500,000
Location:	University of Pittsburgh
Duration:	06/01/21 – 05/31/26
Effort:	0.1 calendar months
Title:	Energy Harvesting and Storage with Gradient Hybrid MOFs

PI:	K. A. Jackson (Central Michigan U.); Co-PIs: J. K. Johnson (Pitt), (with 5 other Co-PIs)
Agency:	U.S. DOE DE-FOA-0002426
Amount:	$560,000 (Pitt share)
Location:	University of Pittsburgh
Duration:	09/01/20 – 08/31/25
Effort:	0.75 calendar months
Title:	FLOSIC: Efficient density functional calculations without self-interaction

Research Products / Acknowledgements:

We published eight peer-reviewed papers in 2023 that acknowledge CRC.

200. Ryan P. McDonnell, Venkata Swaroopa Datta Devulapalli, Tae Hoon Choi, Laura McDonnell, Prasenjit Das, Nathaniel L. Rosi, J. Karl Johnson, Eric Borguet, "Anomalous Infrared Intensity Behavior of Acetonitrile Diffused into UiO-67", *Chem. Mater*., **35**, 8827-8839 (2023). DOI: 10.1021/acs.chemmater.3c00639

199. Mark R. Pederson, Kushantha P. K. Withanage, Zahra Hooshmand, Alex I. Johnson, Tunna Baruah, Yoh Yamamoto, Rajendra R. Zope, Der-You Kao, Priyanka B. Shkula, J. Karl Johnson, Juan E. Peralta and Koblar A. Jackson, "Use of FLOSIC for understanding Anion-Solvent Interactions", *Journal of Chemical Physics*, **159**, 154112 (2023). DOI:10.1063/5.0172300

198. Zoe M. Soilis, Tae Hoon Choi, Joe Brennan, Renee Frontiera, J. Karl Johnson and Nathaniel L. Rosi, "Ligand Chromophore Modification Approach for Predictive Incremental Tuning of MOF Color", *Chemistry of Materials*, **35**, 7741-7749 (2023). DOI: 10.1021/acs.chemmater.3c01603

197. Siddarth K. Achar, Leonardo Bernasconi, Juan J. Alvarez and J. Karl Johnson, “Deep-Learning Potentials for Proton Transport in Double-Sided Graphanol”, *J. Mater. Res*., **38**, 5114-5124 (2023). DOI: 10.1557/s43578-023-01141-3
196. Chinmay V. Mhatre , Jacob J. Wardzala, Priyanka B. Shukla, Mayank Agrawal and J. Karl Johnson, “Calculation of Self, Corrected, and Transport Diffusivities of Isopropyl Alcohol in UiO-66”, *Nanomaterials*, **13**, 1793 (2023). DOI: https://doi.org/10.3390/nano13111793
195. Siddarth K. Achar, Leonardo Bernasconi and J. Karl Johnson, “Machine Learning Electron Density Prediction using Weighted Smooth Overlap of Atomic Positions”, *Nanomaterials*, **13**, 1853 (2023). DOI: 10.3390/nano13121853
194. Siddarth K. Achar, Leonardo Bernasconi, Ruby I. DeMaio, Katlyn R. Howard, J. Karl Johnson, “In Silico Demonstration of Fast Anhydrous Proton Conduction on Graphanol” *ACS Applied Materials and Interfaces*, **15**, 25873-25883 (2023). DOI: 10.1021/acsami.3c04022
193. Priyanka B. Shukla, Prakash Mishra, Tunna Baruah, Rajendra R. Zope, Koblar A. Jackson and J. Karl Johnson “How do self-interaction errors associated with stretched bonds affect barrier height predictions?”, *Journal of Physical Chemistry A, J. Phys. Chem. A*, **127**, 1750−1759 (2023). DOI: 10.1021/acs.jpca.2c07894

Summary Description:

We perform a wide variety of first principles and atomistic empirical calculations to solve problems related to energy and environmental challenges.

Involvement of CRC Consultants:

Leonardo is heavily involved in the machine learning parts of this work. He is coauthor on three of the papers we published in 2023.