



Battelle Memorial Institute, Pacific Northwest Division
 Acting Under Prime Contract DE-AC05-76RL01830
 With the U.S. Department of Energy
 Operating the Pacific Northwest National Laboratory (PNNL) (www.pnnl.gov)

BATTELLE MEMORIAL INSTITUTE, PACIFIC NORTHWEST DIVISION'S CONTRACT NUMBER 738220 Transferring exascale computational chemistry to cloud computing environment and emerging hardware technology (TEC⁴)	
Issued By: Battelle Memorial Institute, Pacific Northwest Division 902 Battelle Boulevard Richland, WA 99352	Contractor: J. Heyrovsky Institute of Physical Chemistry of the Czech Academy of Sciences Dolejšková 2155/3 Prague 8, 18223 Czech Republic (CZE)
Contracts Specialist: Name: [REDACTED] Telephone Number: [REDACTED] Email: [REDACTED]@pnnl.gov	Contractor's Point of Contact: Name: [REDACTED] Telephone Number: +420 [REDACTED] Email: [REDACTED]@jh-inst.cas.cz
Payment Terms: Net 30	Contract Type: Firm Fixed Price
Period of Performance: April 22, 2024 through May 31, 2025	Total Amount of Contract: \$35,000.00 (USD)
Submit Invoices and Invoice/Payment Inquiries To ap.invoices@pnnl.gov. Note: Invoices must list location(s) of service (U.S.: City, State; Foreign: Country).	
Award Battelle hereby awards this Contract to the Contractor subject to acceptance. The rights and obligations of the parties to this Contract are subject to and governed by this document and any documents attached or incorporated by reference.	Contractor Agreement Contractor accepts and agrees to furnish and deliver the items and/or perform the services to the extent stated in this document for the consideration stated in this Contract. The rights and obligations of the parties to this Contract are subject to and governed by this document and any documents attached or incorporated by reference.

Battelle Memorial Institute, Pacific Northwest Division	Contractor shall sign and return a copy of this document
Signature of person authorized to sign	Signature of person authorized to sign
Name [REDACTED]	Name [REDACTED]
Title [REDACTED]	Title [REDACTED]
Senior Contracts Specialist	
Date [REDACTED]	Date

Note: Captions in this document and in Battelle's General Provisions are included for convenience of reference only and in no other way define or delineate any of the provisions hereof or otherwise affect their construction or effect.

1. SCOPE AND PRICING

Scope: Contractor agrees to perform the scope outlined in the attached Statement of Work for this Contract (hereinafter referred to as "Contract").

Deliverable and Payment Schedule: Payment shall be made upon receipt of acceptable deliverables as outlined in the Statement of Work. The payment for all Tasks respectively shall be made upon concurrence by the Technical Oversight Representative (see below) or delegate. The following Payment Schedule shall apply throughout completion of all deliverables.

Deliverables	Due Date	Payment Amount USD
ExaChem-DMRG interface for transferring CC-downfolded interactions.	August 31, 2024	\$ 8,750.00
Modified version of the DMRG to embrace symmetries of the effective interactions represented as two- and four-dimensional tensors.	November 30, 2024	8,750.00
Workflow for performing ExaChem-DMRG simulations on various platforms for various chemical systems and various active spaces.	February 28, 2025	8,750.00
Manuscript reporting on the ExaChem-DMRG workflow. Final report and user manual for the ExaChem-DMRG workflow.	May 31, 2025	\$ 8,750.00

Currency: The currency of this Contract is U.S. Dollars with the amount fixed for the term of the Contract.

2. PERIOD OF PERFORMANCE/DELIVERY

Period of Performance: The period of performance will be in accordance with Page 1 of this Contract.

3. CONTRACTUAL REQUIREMENTS/INFORMATION

4. CONTRACT ADMINISTRATION

Battelle Contracts Specialist: The Battelle Contracts Specialist, [REDACTED] is the sole point of contact for any contractual/administrative communications or questions regarding this acquisition. Contact information is on Page 1.

Technical Oversight Representative: All technical questions should be directed to the Technical Oversight Representative (TOR), [REDACTED] or via email at [REDACTED]. The technical lead is [REDACTED]. The TOR and PNNL's Technical Lead cannot modify this Contract.

Key Personnel: The following named Key Personnel shall be assigned to the performance of the work and shall not be replaced without the prior written approval of the Battelle Contracts Specialist.

- [REDACTED]@jh-inst.cas.cz Principal Investigator
- J [REDACTED]@jh-inst.cas.cz

Lower-tier Subcontractors: Lower-tier Subcontractors require the prior written approval of the Battelle Contracts Specialist.

5. TERMS AND CONDITIONS

The General Provisions for Fixed-Price Other than Commercial Items - Supplies/Services, Form A-409.32-FP dated April 2024, apply and may be viewed at <https://www.pnnl.gov/procurement/documents>.

6. CONTRACT ATTACHMENTS

In addition to the above, the Contract consists of:

- Statement of Work, dated April 22, 2024
- Representations and Certifications, dated April 9, 2024

7. ENTIRE AGREEMENT

This Contract contains the entire agreement and understanding between the parties, and there are no agreements, understandings or representations not set forth or incorporated by reference herein. This Contract supersedes all prior proposals, understandings and agreements, whether oral or written, between the parties with respect to the subject matter hereof. No subsequent Modifications of this Contract shall be of any force or effect unless in writing by authorized representatives of each party to this Contract. No communications, written or oral, by other than a Battelle Contracts Specialist shall be effective to modify or otherwise affect the provisions of this Contract.

