ABHISHEK KHEDKAR, PhD

POST DOCTORAL RESEARCH ASSOCIATE
KING'S COLLEGE LONDON (KCL)

CONTACT INFO

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CAREER STATEMENT

I am a hands-on, principled scientific software developer (Python, C++ and Fortran) experienced in designing, programming, and testing software across a variety of platforms. I am continuously updating my skills and have worked on numerous implementation, library-interfacing, compilation, optimization projects, from concept to completion.

SKILLS

- **Programming:** Python (6+ years), Fortran (3 years), C/C++ (4+ years), Julia (basic), Bash (11+ years), LaTeX, CUDA (basic), OpenMP, MPI, Boost
- **Tools:** Linux, Git, SVN, PyTorch (basic), TensorFlow (basic), gdb, Maqao, Scalene, Numba, GitHub actions, Qiskit (basic)
- **Simulation Packages:** PySCF, Vayesta, IPie, Quantum Espresso, Quantum Package, BLOCK (DMRG), TurboRVB, ORCA, Gaussian, Block2 (Python), MOLBLOCK

EXPERIENCE

February 2023 - present
Post-doctoral Research Associate, **Theoretical Physics**
King's College London, London, UK

- Developed, tested, and benchmarked local variants of coupled cluster methods for molecular and extended systems within the Vayesta Python package for quantum embedding calculations.
- Contributed to maintenance, documentation, and bug fixing as one of the developers of Vayesta.
- Improved and tested the Python interface pygnme for libgnme, a C++ library for evaluating non-orthogonal matrix elements in electronic structure.

October 2021 - February 2023
Post-doctoral Research Associate, **Quantum Condensed Matter Theory**
SISSA, Trieste, Trieste, Italy

- Contributed various features to the TurboRVB Quantum Monte Carlo package written in Fortran, including a fast inverse-update, hybrid OpenMP-MPI parallelized version for walkers in Monte Carlo simulations, and a streamlined CMake build system for various architectures.
- Implemented higher-order, mixed derivatives of Jastrow-Geminal and Pfaffian wavefunctions needed for backflow transformed wave function in Variational Quantum Monte Carlo.
- Conducted extensive scaling and profiling analyses for TurboRVB (Quantum Material Simulation package written in Fortran), resulting in a 18% reduction in processing time and improved overall system performance in collaboration with HPC experts at UVSQ (Uni-Versaille).
- Worked closely with the core team of QMCkl developers (Uni-Toulouse) to interface with the TurboRVB package and utilize high-performance math kernels.

October 2020 - September 2021
Research Associate, **Theoretical Chemistry**
Ruhr University Bochum (RUB), Bochum, Germany

- Developed, tested, and benchmarked an active orbital space selection scheme named "ASS1ST" based on multireference perturbation theory (DMRG-SC-NEVPT2) in the multireference quantum chemistry package MOLBLOCK, written in C++.
- Implemented an MPI-parallelized and highly optimized version of the ASS1ST method for ground and excited states for molecular systems, enabling the investigation of previously intractable systems.

EDUCATION

2020
PhD, Theoretical Chemistry
Max Planck Institute for Coal Research /
Ruhr University Bochum, Germany
Supervisor: Prof. Michael Roemelt

- Contributed features, improved integral handling, and build system (GNU make) as one of the developers of MOLBLOCK C++ multireference quantum chemistry package.
- Worked closely with experimental groups and spectroscopists to validate theoretical findings.
- Ensured the organization and accessibility of critical scientific data sets through comprehensive Research Data Management in adherence to the norms of the German Chemical Society (GDCh),

2015
M. Sc. (Integrated), Chemistry
IIT Kanpur, India
Supervisor: Prof. Shridhar R. Gadre

PUBLICATIONS

1. Iffland, L., Khedkar, A., Petuker, A., Lieb, M., Wittkamp, F., van Gastel, M., Roemelt, M., & Apfel, U.-P. (2019). Solvent-controlled co2 reduction by a triphos–iron hydride complex. *Organometallics*, *38*(2), 289–299

2. Khedkar, A., & Roemelt, M. (2019). Active space selection based on natural orbital occupation numbers from n-electron valence perturbation theory. *Journal of Chemical Theory and Computation*, *15*(6), 3522–3536

3. Khedkar, A., & Roemelt, M. (2020a). An ab initio multireference study of reductive eliminations from organoferrates (iii) in the gas-phase: It is all about the spin state. *Physical Chemistry Chemical Physics*, *22*(31), 17677–17686

4. Khedkar, A., & Roemelt, M. (2020b). Extending the ass1st active space selection scheme to large molecules and excited states. *Journal of Chemical Theory and Computation*, *16*(8), 4993–5005

5. Khedkar, A., & Roemelt, M. (2021). Modern multireference methods and their application in transition metal chemistry. *Physical Chemistry Chemical Physics*, *23*(32), 17097–17112