Simplifying Multilevel Quantum Chemistry Procedures through Psi4 and QCArchive

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Abstract: The Psi4 quantum chemistry (QC) program is reworking its outer Python layer to facilitate high-throughput computing. For users, this allows naturally parallel procedures such as composite methods or many-body routines to run in parallel with minimal changes to the input. Central to this effort is interfacing with The Molecular Sciences Software Institute's Quantum Chemistry Archive (QCA) project to provide database storage and query and promote standard interfaces, QCSchema, for communication between software projects in the field. Capabilities to call Psi4 and other QC programs through increasingly uniform input suitable for software generation will also be presented.