Molpro

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Molpro is a general purpose quantum chemistry software package with a long development history. It was originally focused on accurate wavefunction calculations for small molecules but now has many additional distinctive capabilities that include, inter alia, local correlation approximations combined with explicit correlation, highly efficient implementations of single-reference correlation methods, robust and efficient multireference methods for large molecules, projection embedding, and anharmonic vibrational spectra. In addition to conventional input-file specification of calculations, Molpro calculations can now be specified and analyzed via a graphical user interface and through a Python framework.

Recent developments, including improved density functional quadrature, will be described.

References

https://www.molpro.net

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