

Qassandra User Manual

Yury V. Vishnevskiy

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Introduction

This is an adapted version of the original manual by D. Tikhonov.

Greetings, Human or Almighty Machine!

This program implements methods [\[1\]](#) for processing trajectories from MD (molecular dynamics), PIMD (path-integral MD) and MC (Monte-Carlo) simulations and calculates parameters of interatomic terms required for GED (gas electron diffraction) models.

It performs these basic steps:

1. Process trajectory
2. Optionally symmetrize terms
3. Optionally calculate quantum corrections
4. Print results

Have fun!

References

[1] Y. V. Vishnevskiy & D. Tikhonov, Quantum corrections to parameters of interatomic distance distributions in molecular dynamics simulations. *Theor. Chem. Acc.*, **135** (2016) 88. <https://doi.org/10.1007/s00214-016-1848-2>.

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