

Generation of optimized structures using Particle Swarn Optimization (PSO)

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1 Introduction

For as long as both theoretical and technological progress entitled scientists to do, there has been a wide interest to understand the nanoscopic scale of matter. Indeed, doing so makes it possible to understand the processes and the results of changement inside the matter (phase transition)

This report, based on the publication from Robinson et al. [1], tackles the application of a generalized optimization algorithm (Particle Swarn Optimization) for the purposes of potential energy surfaces exploration and the determination of the optimized geometry for particular conditions.

2 Particle Swarn Optimization

Particle Swarm Optimization (PSO) is a population-based optimization algorithm that simulates the social behavior of birds or insects, such as flocking or swarming.

3 Comparison to other generation methods

4 Conclusion

References

- [1] NADEN ROBINSON, V., MARQUÉS, M., WANG, Y., MA, Y., AND HERMANN, A. Novel phases in ammonia-water mixtures under pressure. *The Journal of Chemical Physics* 149, 23 (2018), 234501.