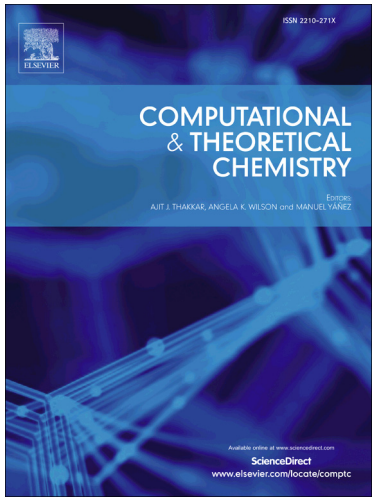

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Jack Yang, Mark P. Waller

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A Hybrid Dimer Swarm Optimizer

Jack Yang and Mark P. Waller*

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Abstract

Here we present a dimer swarm optimizer (DSO) that hybridizes a particle swarm optimizer (PSO) [*J. Chem. Theory Comput.*, **9**, 2137 (2013)] and the stochastic surface walking SSW [*J. Chem. Theory Comput.*, **9**, 1838 (2013)] method. The DSO has additional biasing modes in the dimer rotation step in order to drive an individual towards the global, iteration and neighboring best particles in the swarm. The DSO was augmented with an adaptive Gaussian half-width and Monte Carlo temperature scheme. DSO has been validated on three LJ_n clusters of increasing sizes (n=31, 38 and 55).

Keywords: Global optimization, Particle swarm, Monte Carlo

1 Introduction

Geometry optimization is one of the cornerstones of computational chemistry.[1] The most common geometry optimizers currently employed in modern computational chemistry packages are gradient-based[2–4] and therefore can typically only locate local minima on a potential energy surface (PES). Their success heavily relies upon the availability of a good starting structure, which can sometimes be obtained from experimental studies (e.g. X-ray diffraction or NMR studies). When no experimental structure is available, a starting guess can be constructed using chemical intuition, however, this soon becomes intractable when the molecular complexity increases. These shortcomings in traditional gradient based optimizers can be overcome by global optimizers,[5–10] which are, to a degree, independent from the starting point or at least not completely hindered by the energy barriers. Furthermore, a single structure is a very crude approximation for the real system, which makes it quite difficult to understand the thermodynamic properties of the system from a statistical point of view.[11–13] Therefore, another advantage of global optimizers is their ability to collect a range of low energy minima, which can be used in more comprehensive computational studies.

Introducing stochastic components into the optimization procedure is important to enable the optimization algorithm to be more explorative.[14] The recently proposed Stochastic

*Organisch-Chemisches Institut, Westfälische Wilhelms-Universität Münster, Corrensstraße 40, 48149, Münster, Germany. Email: m.waller@uni-muenster.de