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Christensen, Rasmus; Sørensen, Søren Strandkov; Liu, Han; Li, Kevin; Bauchy, Mathieu; Smedskjær, Morten Mattrup

Publication date:
2022

Document Version
Other version

[Link to publication from Aalborg University](#)

Citation for published version (APA):

Christensen, R., Sørensen, S. S., Liu, H., Li, K., Bauchy, M., & Smedskjær, M. M. (2022). *Interatomic potential parameterization using particle swarm optimization: Case study of glassy silica*. Poster presented at 26th International Congress on Glass, Berlin, Germany.

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Interatomic potential parameterization using particle swarm optimization: Case study of glassy silica

R. Christensen^{1*}, S. S. Sørensen¹, H. Liu², K. Li², M. Bauchy², M. M. Smedskjaer¹

¹ Department of Chemistry and Bioscience, Aalborg University, DK-9220 Aalborg, Denmark.,

² Department of Civil and Environmental Engineering, University of California, Los Angeles, California 90095, USA.

*rasmusc@bio.aau.dk

Classical molecular dynamics simulations of glassy materials rely on the availability of accurate yet computationally efficient interatomic force fields. The parameterization of new potentials remains challenging due to the non-convex nature of the accompanying optimization problem, which renders the traditional optimization methods inefficient or subject to bias. In this study, we present a new parameterization method based on particle swarm optimization (PSO), which is a stochastic population-based optimization method. Using glassy silica as a case study, we introduce two interatomic potentials using PSO, which are parameterized so as to match structural features obtained from ab initio simulations and experimental neutron diffraction data. We find that the PSO algorithm is highly efficient at searching for and identifying viable potential parameters that reproduce the structural features used as the target in the parameterization. The presented approach is very general and can be easily applied to other interatomic potential parameterization schemes.