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

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We present a new method based on particle swarm optimization (PSO) for parameterization of interatomic potentials. Using glassy silica as a case study, we parameterize two interatomic potentials based on structural features obtained from ab initio simulations and experimental neutron diffraction data.

<u>Reference</u>: Christensen R., Sørensen S. S., Liu H., Li K., Bauchy M., Smedskjaer M. M. Interatomic potential parameterization using particle swarm optimization: Case study of glassy silica. *Journal of Chemical Physics* **154**, 134505 (2021).