Catchment basin self-avoiding simulated annealing for global optimization method MINGHAI LI, XI LIN, Boston University, Mechainical Engineering Dept — We develop a generic global minimization algorithm which can escape from catchment basins on the 3N-dimensional potential energy surface. The essential idea is to combine the simulated annealing with our recently developed history-penalized basin filling method. In this work, we present the most energetically favorable configurations of all Lennard-Jones (LJ) clusters up to 60 atoms, including the most challenging 38-atom cluster which the conventional simulated annealing algorithm failed. In addition, we report for the first time the most energetically favorable configurations for polymer chains consisting of up to 60 LJ monomers and their potential energy disconnectivity graphs.

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