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Lattice Optimization with Adaptive Tempering Simulations XIAO DONG, ESTELA BLAISTEN-BAROJAS, School of Computational Sciences, George Mason University, Fairfax, VA 22030 — An Adaptive Tempering optimization based on multi-canonical Monte Carlo is proposed to optimize the structure of the solid crystal obtained at low temperatures in an annealing process. The parameters that link the sub-canonical ensembles are adapted progressively during the simulation. Solidification from a liquid system can be achieved through this method fairly fast. Tests of the method were done on Lennard-Jones (LJ) liquid systems of various computational box sizes with periodic boundary conditions. Quenching from high temperature, the systems crystallized with few defects in a single pass of the tempering. The only observed defects were one or two stacking faults. The method was additionally tested on LJ clusters, for which the global minimum structure was obtained at the end of the quench.

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