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Genarris: Parallelized Configuration Space Screening of Molecular Crystals Aided by a Harris Approximation XIAYUE LI, Tulane University, FARREN CURTIS, Carnegie Mellon University, CHRISTOPH SCHOBER, Technical University of Munich, ALVARO VAZQUEZ-MAYAGOITIA, Argonne National Laboratory, HARALD OBERHOFER, Technical University of Munich, NOA MAROM, Carnegie Mellon University — Genarris is a Python-based package for parallelized configuration space screening for crystals of rigid molecules. Genarris is designed to rapidly create a low-energy and high-diversity initial pool for further crystal structure prediction based on a genetic algorithm. Genarris generates random structures with physical constraints by applying space group symmetries and customizable closeness checks. For fast total energy evaluations, Genarris employs a Harris approximation, whereby the total charge density of a molecular crystal is constructed via superposition of single molecule densities. Dispersion-corrected density functional theory (DFT) is then used with the Harris density as input to compute the total energy in one iteration. To balance the need for quality and diversity, the pool is enriched with structures only meeting looser closeness criteria. The lowest energy structures are then selected from clusters of similar structures, found by a $k-$means algorithm based on a radial distribution function descriptor.

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