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Computational Discovery of Materials Using the Firefly Algorithm[1] GUILLERMO AVENDAO-FRANCO, ALDO ROMERO, West Virginia University — Our current ability to model physical phenomena accurately, the increase computational power and better algorithms are the driving forces behind the computational discovery and design of novel materials, allowing for virtual characterization before their realization in the laboratory. We present the implementation of a novel firefly algorithm, a population-based algorithm for global optimization for searching the structure/composition space. This novel computation-intensive approach naturally take advantage of concurrency, targeted exploration and still keeping enough diversity. We apply the new method in both periodic and non-periodic structures and we present the implementation challenges and solutions to improve efficiency. The implementation makes use of computational materials databases and network analysis to optimize the search and get insights about the geometric structure of local minima on the energy landscape. The method has been implemented in our software PyChemia, an open-source package for materials discovery.

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