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Global structure optimization of complex systems CAI-ZHUANG WANG, MIN JI, KAI-MING HO, Ames Laboratory, U.S. DOE and Department of Physics and Astronomy, Iowa State University, Ames, Iowa 50011, USA — Finding the global minimum structure of complex condensed matter systems is a long-standing challenge in computational physics. Genetic algorithm, basin-hopping or simulated annealing are popular methods to explore the configurational space. Here we applied these methods to periodical systems such as crystalline solids and alloys, metal on semiconductor surfaces and interface structures. Novel structures can be revealed in complex and multicomponent systems. The efficiency of different search strategies is also discussed.

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