Nature-inspired algorithms for surface structure predictions

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Predicting the atomic structure of materials and investigating the emergent physical and chemical property is the primary challenge in the field of nanoscience. Currently, most atomic structures used in the field of computational surface science are often represented by a low Miller index surface slab, lacking critical structural features like steps, facets, (co)adsorbates, and surface reconstructions. Another commonly used approach in designing the surfaces is based on the conventional knowledge, e.g. using only the surface with the lowest surface energy in vacuum, though these surfaces may be less interesting. Nature-inspired algorithms such as particle swarm optimization (PSO) and genetic algorithm (GA), which mimics and adopts the characteristic behavior found in nature to solve optimization problem, is in a limelight as an alternative method to survey vast configurational space without confronting the limits mentioned above. Especially, Firefly algorithm, one class of nature-inspired algorithm, has been suggested to outperform other algorithms in finding many interesting surface structures due to its automatic subgrouping around the local minima. In this talk, surface structure predictions based on the nature-inspired algorithms will be presented, as well as the efficiency and reliability of algorithms will be discussed.