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Materials Discovery via CALYPSO Methodology

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Materials design has been the subject of topical interests in materials and physical sciences for long. Atomistic structures of materials occupy a central and often critical role, when establishing a correspondence between materials performance and their basic compositions. Theoretical prediction of atomistic structures of materials with the only given information of chemical compositions becomes crucially important, but it is extremely difficult as it basically involves in classifying a huge number of energy minima on the lattice energy surface. To tackle the problems, we have developed an efficient CALYPSO (Crystal structural AnLYsis by Particle Swarm Optimization) approach [1-2] for structure prediction from scratch based on particle swarm optimization algorithm by taking the advantage of swarm intelligence and the spirit of structures smart learning. The method has been coded into CALYPSO software (http://www.calypso.cn) which is free for academic use. Currently, CALYPSO method is able to predict structures of three-dimensional crystals, isolated clusters or molecules [3], surface reconstructions [4], and two-dimensional layers [5]. The applications of CALYPSO into purposed materials design of layered materials [6], high-pressure superconductors [7], and superhard materials [8] were successfully made. Our design of superhard materials [8] introduced a useful scheme, where the hardness value has been employed as the fitness function. This strategy might also be applicable into design of materials with other desired functional properties (e.g., thermoelectric figure of merit, topological Z2 number, etc.). For such a structural design, a well-understood structure to property formulation is required, by which functional properties of materials can be easily acquired at given structures. An emergent application is seen on design of photocatalyst materials.

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