

Atomistic Structure Prediction via Swarm Intelligence Algorithms

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Knowledge of atomistic structures is essential if the properties of materials are to be understood and exploited, particularly when establishing a correspondence between materials performance and their chemical compositions. Precise prediction of atomistic structures with the given information of chemical compositions is highly desirable, but it is extremely difficult as it basically involves in exploring a huge number of energy minima on the high-dimensional potential energy surface. There is an urge on development of global optimization algorithms on efficient exploration of energy surface to identify the global stable structure.

We have developed an efficient CALYPSO structure prediction approach [1-2] via multi-objective swarm-intelligence optimization algorithms by taking the advantage of structures smart learning where both particle swarm optimization and artificial bee colony algorithms are employed (See more information at <http://www.calypso.cn>). The method has been widely used by more than 1600 users to design multi-dimensional structures ranging from 3D bulk crystals to 0D nanoclusters, 2D layers and surfaces, etc [3-5]. Functionality-driven inverse design of electrified, superhard, and optical materials are also feasible [6].

CALYPSO has played a leading role in major high-pressure experimental discoveries. Predicted chemical reactions of Fe/Ni and Xe at the conditions of Earth core [7] and its experimental confirmation might provide a possible solution on “missing Xe paradox” towards to the Xe storage in the Earth Core. Our prediction of high-T_c superconductivity of H₂S [8] has initiated the exciting experimental discovery of record high 200 K superconductivity on highly compressed H₂S.

References:

- [1] Y. Wang, J. Lv, L. Zhu, and Y. Ma, Phys. Rev. B 82, 094116 (2010).
- [2] Y. Wang, J. Lv, L. Zhu, and Y. Ma, Comput. Phys. Commun. 183, 2063 (2012).
- [3] J. Lv, Y. Wang, L. Zhu, and Y. Ma, J. Chem. Phys. 137, 084104 (2012).
- [4] S. Lu, Y. Wang, H. Liu, M. Miao, and Y. Ma, Nature Commun. 5, 3666 (2014).
- [5] Y. Wang, et al., J. Chem. Phys. 137, 224108 (2012).
- [6] X. Zhang, et al., J. Chem. Phys. 138, 114101 (2013).
- [7] L. Zhu, H. Liu, C. Pickard, G. Zou, and Y. Ma, Nature Chem. 6, 644 (2014).

[8] Y. Li, J. Hao, H. Liu, Y. Li, and Y. Ma, *J. Chem. Phys.* **140**, 174712 (2014).