# Materials by Design Via Simulations of Atomistic Structures

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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 basic composition. An ultimate goal of materials research is able to design materials by wish. For doing so, a precise simulation of atomistic structures of materials with the only given information of chemical composition, without relying on any prior known structure knowledge, is highly desirable, but it is extremely difficult as it involves in simulating a vast number of possible structures on the entire structure space.

We have developed a CALYPSO approach [1-2] for a precise simulation of atomistic structure of materials from "scratch" via multi-objective swarm-intelligence optimization algorithms where both particle swarm optimization and artificial bee colony algorithm are employed. The method has been coded into the CALYPSO software (http://www.calypso.cn) that has been widely used by more than 3,200 users from 73 different countries to design multi-dimensional materials ranging from 3D bulk materials to 0D and 2D materials, etc [3-4]. Functionality-driven inverse design of electride and superhard materials are now also feasible [5-6].

In this talk, I will give a short introduction to the principle of CALYPSO method and present examples for materials by design via simulation of atomistic structures using CALYPSO code. Particular emphasis will be placed on the discussions of recent breakthrough findings of near room-temperature (300K) superconductors among superhydrides (e.g., $LaH_{10}$ at $T_c$ = 260 K) stabilized at high pressure where CALYPSO has played a leading role in directing the experimental discoveries. The design-orientated findings of clathrate superhydride ($CaH_6$, $YH_6$, $YH_9$, and $LaH_{10}$) [7-9] showcase a class of best-ever known superconductors in term of $T_c$ values. The work opens up the possibility of finding a room-temperature superconductor, which is a century long-held dream of mankind.

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