北京大学量子材料科学中心
International Center for Quantum Materials, PKU

Weekly Seminar

CALYPSO晶体结构计算方法与软件

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Time: 3:00 pm, Nov. 16, 2022 (Wednesday)

时间：2022年11月16日 （周三）下午3:00

腾讯会议链接: https://meeting.tencent.com/dm/5EfFkatva5Wq

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摘要

计算科学目前步入快速发展时期，部分计算已经实现了精准预测，在多项原始创新研究上起到了引领作用。计算强烈依赖于计算方法和软件的创新，但我国自主创新的科学计算软件，特别是具有国际影响力的计算软件，寥寥无几。为了提升我国在计算领域的核心竞争力，亟需研发自主创新的科学计算软件。本报告主要介绍我课题组发展的以CALYPSO命名的晶体结构计算方法和软件（依据化学组分就可以计算出晶体结构，详见http://www.calypso.cn）[1,2]。该方法和软件已经被70余个国家的4000余位同行采用开展结构设计研究，在物理、化学、材料、地学等多个学科领域解决了一系列科学问题，所取得的成果已经在PRL、PNAS等期刊发表了1500余篇学术论文。

参考文献：

1. Yanchao Wang, Jian Lv, Li Zhu, and Yanming Ma, Phys. Rev. B 82, 094116 (2010)
2. Yanchao Wang, Jian Lv, Li Zhu, and Yanming Ma, Comput. Phys. Commun. 183, 2063 (2012)

报告人简介

Prof. Yanming Ma (http://mym.calypso.cn) received his Ph.D (2001) in Jilin University, China, and then worked as a postdoctoral researcher at the Steacie Institute for Molecular Sciences, National Research Council of Canada (2002-2004) and Laboratory of Crystallography in ETH, Switzerland (2006-2008). He is currently a distinguished Au-Chin Tang Professor in College of Physics, and vice President of Jilin University. His research interests mainly focus on development of simulation methods (e.g., CALYPSO at http://www.calypso.cn) on crystal structure prediction and large-scale electronic structure calculations of materials, and the use of these developed methods for design of materials (e.g., hydrogen-rich superconductors and superhard materials, etc) under high pressure conditions. He has published >360 Peer-reviewed papers with more than 24,000 citations, given more than 100 invited talks in conferences and universities, and is the recipient of a highly cited researcher (2017-2021) from Clarivate Analytics. He received the Jamieson Award for High Pressure Science and Technology (2001) and the very first Walter Kohn Prize for Quantum-mechanical Materials and Molecular Modeling (2016).