凝聚态物理-北京大学论坛

北京大学物理学院凝聚态物理与材料物理研究所
2023年第9期（No.561 since 2001）

Numerically accurate all-Electron GW approach to electronic band structure of materials

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时间：4月20日（星期四）15:00—16:30

地点：北京大学物理楼西202报告厅

报告人简介（About speaker）：蒋鸿，1998年获得北京大学理学学士学位，2003年获得北京大学物理化学专业理学博士学位。科研经历包括2001年-2004年美国杜克大学访问学生/博士后，2004年-2006年德国法兰克福大学博士后，2006年-2009年德国柏林弗里兹-哈勃研究所博士后。2008年底入职北京大学化学与分子工程学院，现为研究员(长聘副教授)。主要研究兴趣是发展针对材料体系的电子结构理论方法和计算程序，并将其应用于重要新材料的理论研究。

摘要（Abstract）：Many-body perturbation theory in the GW approximation has been regarded as the most accurate and robust first-principles approach to electronic band structure of insulating materials. In this talk I will address the challenges of numerically accurate GW calculation based on our recent systematic investigation of the effects of including high-energy local orbitals (HLOs) in the linearized augmented plane waves (LAPW)-based all-electron GW calculations for both weakly and strongly correlated materials [1-5]. We found that both the accuracy of unoccupied states and the completeness in the summation of states are crucial for numerically accurate GW calculations, which can provide important clues to the construction of more accurate pseudopotentials and the development of new approaches that eliminate or reduce the efforts necessary for the summation of unoccupied states.

[1] H. Jiang et al. Computer Phys. Commun.,2013, 184:348.

[2] H. Jiang and P. Blaha, Phys. Rev. B, 2016, 93:115203.

[3] M.-Y. Zhang and H. Jiang, Phys. Rev. B. 2019, 100: 205123.

[4] H. Jiang, Phys. Rev. B, 2018, 97:245132.

[5] M.-Y. Zhang and H. Jiang, Frontiers of Chemistry, 2021, 9, 747972.

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http://www.phy.pku.edu.cn/icmp/xsjl/njtwl__bjdxlt.htm