量子材料科学中心
International Center for Quantum Materials

Weekly Seminar

First-principles electronic structure methods, random-phase approximation, and beyond

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Time: 4:00 pm, April.3, 2013 (Wednesday)
时间： 2013年4月3日（周三）下午 4:00
Venue: Conference Room A (607), No. 5 Science Building
地点： 理科五号楼607会议室

Abstract

I will first give a brief overview of major first-principles methods in the market today used for electronic structure calculations. Then I will highlight one approach, called random-phase approximation (RPA) [1], that gets increasingly popular in recent years for ground-state total-energy calculations in chemistry and condensed-matter physics. Remarks will be given on its success as well as remaining shortcomings. As a further extension of RPA, I will introduce the renormalized second-oder perturbation theory (rPT2) [2], that combines RPA, second-order screened exchange (SOSEX), and renormalized single excitation (rSE) [3,4] contributions. Extensive benchmarks showed that rPT2 represents "the most balanced approach" for different electronic situations and is a promising candidate for general-purpose electronic-structure calculations. All these developments and benchmark calculations were carried out in and with the FHI-aims code package [5,6].

[1] X. Ren, P. Rinke, C. Joas, M. Scheffler, J. Mater. Sci. 47, 7447 (2012).
[2] X. Ren, P. Rinke, G. E. Scuseria, and M. Scheffler, arXiv:1212.3674v2 (2013).
[3] X. Ren, A. Tkatchenko, P. Rinke, and M. Scheffler, Phys. Rev. Lett. 106, 153003 (2011)
[4] J. Paier, X. Ren, P. Rinke, G. E. Scuseria, A. Grueneis, G. Kresse, and M. Scheffler, New J. Phys. 14, 043002 (2012).
[5] V. Blum, R. Gehrke, F. Hanke, P. Havu, V. Havu, X. Ren, K. Reuter, M. Scheffler, Comp. Phys. Comm. 180, 2175 (2009).
[6] X. Ren, P. Rinke, V. Blum, J. Wieferink, A. Tkatchenko, A. Sanfilippo, K. Reuter, M. Scheffler, New J. Phys. 14, 053020 (2012).

About the Speaker

任新国，男，2006年毕业于德国Augsburg大学物理研究所，获博士学位。2006-2012年在德国柏林Fritz-Haber研究所做博士后研究。2013起任中国科技大学量子信息重点实验室特任研究员。主要研究方向是基于第一性原理的电子结构方法的发展，程序化，和在实际材料中的应用。

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