武汉物数所理论交叉学术交流系列报告

(第一一一期)

Spectroscopy, dynamics & kinetics on high-level full-dimensional ab initio Potential Energy Surfaces (PES)

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2014年12月19日(周五) 上午10:30-12:00
频标楼4楼报告厅

报告人简介：李军博士, 2002-2006年四川大学本科; 2006-2011年四川大学博士(指导教授:李象远). 2009-2010年台湾国立交通大学应化系访问学者(指导教授:林圣贤). 2011-2014年美国新墨西哥大学化学系博士后研究员(指导教授:郭华). 2014年9月开始在重庆大学化学化工学院工作, 特聘研究员, 博士生导师. 研究方向为理论化学和计算化学, 主要包括: 势能面, 反应热/动力学, 反应动态学, 光化学等. 已发表SCI论文共44篇.

Abstract: **In principle, once the PES is known, all the spectroscopy and dynamical/kinetics properties can be calculated. As a result, much efforts have been devoted to developing accurate and efficient PESs. Recently, we proposed the approach of permutation invariant polynomials neural network (PIP-NN), in which the permutation invariant polynomials (PIP) was used as symmetry functions in the input vector of neural network (NN). It has been applied to several examples, including FH_2O (A_2BC), OH_2O (A_2B_2), H_3O (A_3B), N_4 (A_4), CH_4 (A_4B), CH_2OO (A_2B_2C), etc. The resulting PIP-NN PESs typically have very small root mean square deviations (RMSDs), general on the order of meV. Spectroscopy and dynamical/kinetics calculations are performed on these PIP-NN PESs, and generally the agreement with the experiment is excellent. With the rapid advances in electronic structure theory, PESs of complex systems can now be constructed efficiently and accurately, and the simulations are more reliable with these accurate PESs.**

主办单位:武汉物数所理论与交叉研究部