Academic Presentations in Physics

物理学系列学术报告

报告题目：内层电子电离态的高精度运动方程耦合簇和 Delta 耦合簇方法

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报告时间：2021 年 6 月 11 日（周五）上午 10:00

报告地点：长安校区物理楼 852 报告厅

报告摘要：

Benchmark scalar-relativistic core–valence-separated (CVS) equation-of-motion coupled-cluster ionization potential (EOMIP-CC) calculations of 21 K-edge ionization energies of C, O, N, and F in 14 molecules are presented [1]. The CVS-EOMIP-CC methods are shown to be numerically more stable and more accurate than the parent EOMIP-CC methods. The superior performance of the CVS scheme is attributed to the exclusion of spurious couplings between core-ionized states and valence continuum states. Systematic improvement of computed K-edge ionization energies within the CVS-EOMIP-CC hierarchy, including the CC singles and doubles (CCSD) method, the CC singles, doubles, and triples (CCSDT) method, and the CC singles, doubles, triples, and quadruples (CCSDTQ) [2] method, is demonstrated, with CCSDTQ yielding essentially quantitative results. Maximum absolute deviations (MaxAD) between best computed and experimental results amount to 0.23 eV. The corresponding standard deviations (SD) is only 0.10 eV. Delta-coupled-cluster theory (ΔCC) methods for calculations of *1s* core-ionization energies and hetero-site double core ionization energies for the small molecules which are composed of the first long row elements are also presented and studied [3,4]. On the basis of systematic convergence of computational results with respect to basis-set effect, electron correlation and correction to the core-valence separation approximation, ΔCCSD(T) calculations have been shown to be capable of providing accurate single core ionization energies with a MaxAD of 0.22 eV and SD of 0.13 eV as well as double core ionization energies with remaining errors estimated to be below 0.3 eV. We consider the CVS-EOM-CC and ΔCC are reliable and robustness tools to facilitate experimental studies of single and double core-ionized states that are involved in X-ray pump/X-ray probe studies of electronic and molecular dynamics following inner shell ionization or excitation.

[1]. J. Liu, D. Matthews, S. Coriani, L. Cheng. *J. Chem. Theory Comput.,* 2019, **15** (3), 1642-1651.

[2]. D. Matthews, and J. F. Stanton, *J. Chem. Phys.* 2015, **142** (6), 064108.

[3]. X. Zheng, L. Cheng. *J. Chem. Theory Comput.*, 2019, **15** (9), 4945-4955.

[4]. X. Zheng, J. Liu, G. Doumy, L. Young, L. Cheng. *J. Phys. Chem. A* 2020, **124** (22), 4413-4426.

报告人简介：刘俊孜 2014 年毕业于北京大学化学与分子工程学院，获物理化学博士学位。随后分别在中国科学院化学研究所和 Johns Hopkins University 从事博士后研究。2021 年被北京科技大学化学与生物工程学院聘为特聘副教授。现已在高水平期刊发表学术论文 17 篇。研究兴趣主要集中于分子体系激发态的量子化学方法发展和应用，目前的研究方向是发展基于酉耦合簇理论的极化传播子理论。此外，对使用相对论运动方程耦合簇方法和 Delta 耦合簇方法进行内层电子激发态 (core excitation) 计算和 X 射线光谱的模拟也有深入研究。

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