Applied Math Ph.D. Seminar

FUDAN UNIVERSITY

Basis-set-error-free RPA correlation energy based on Sternheimer equation

Speaker: Hao Peng(Chinese Academy of Sciences)

Time: 2024-05-09, 16:10 to 17:00

Location: Rm 1801, Guanghua East Tower

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Abstract: The problem of basis set incompleteness error(BSIE) in correlation calculation methods (such as RPA, GW, MP2, etc.) has received widespread attention. Essentially, BSIE originates from the perturbation expansion, which requires a complete set of eigenfunctions for non interacting Hamiltonian. Although using correlated consistent basis sets to extrapolate to the complete basis set (CBS) limit can effectively eliminate BSIE, accurate basis set limits are still difficult to obtain. The accuracy of the extrapolation results also needs to be confirmed. Our research aims to provide the RPA correlation energy without BSIE, in order to provide the correct CBS. This can provide us with some reference results and also evaluate the accuracy of common correlation calculation methods in quantum chemistry.