Simulating, Modeling, and Analyzing 2D IR-Raman and 2D electronic-vibrational Spectroscopies



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报告摘要:

Understanding dynamics in complex environments of molecular liquids and biological systems has been a central topic of investigation in chemistry and biology, because many important chemical processes occur exclusively in such media. The key feature of this system is that it describes irreversible dynamics refers to open quantum dynamics through which the primary system evolves toward the thermal equilibrium state at finite temperature. Our group have been working on this problem on the basis of the reduced equations of motion approach. In this talk, I overview our latest results for the following three topics.

- 1) 2D IR-Raman spectroscopy for liquid water.
- 2) 2D electronic vibrational spectroscopies (2DEVS) for non-adiabatic transition system.
- 3) 2D rotational spectroscopy for 3D quantum rotor system.

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