THE GEODYNAMICS SEMINAR

№ 652

Non-Equilibrium Dynamics in Organic Systems: Insights from Molecular Dynamics

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2026.2.13 (Fri.) 16:30 ~

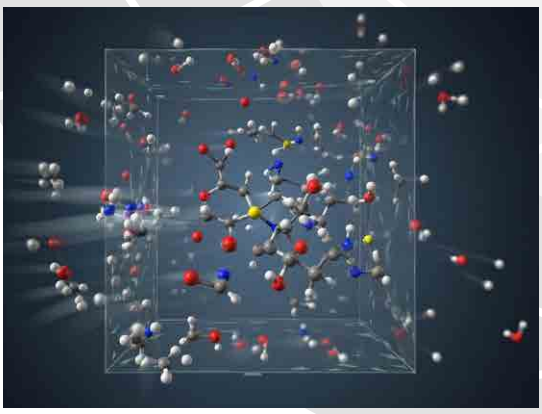
Venue: Meeting Room #486

Science Research Bldg. 1, 4th floor.
Ehime Univ.

We report on our recent studies of excited-state dynamics in organic molecules using first-principles molecular dynamics incorporating nonadiabatic effects. Energy transfer processes in organic systems, such as excited electron and hole transport, are intimately coupled to molecular motions. In this seminar, we present a detailed analysis of energy transfer mechanisms by simultaneously tracking electronic dynamics and nuclear motion within a first-principles framework. This approach enables us to clarify which specific molecular motions play key roles in mediating energy transport. In addition to energy transfer phenomena, we will briefly introduce our recent work on nonequilibrium dynamics conducted in our research group.

Keywords

1. Non-Equilibrium phenomena
2. Molecular dynamics
3. Excited states



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