Quantum Chemistry for Excited States

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Quantum chemistry has been established as a useful approach to elucidate the mechanism of various chemical phenomena and to design molecular materials or catalytic systems. Theories and their computational algorithm for molecular excited states have also been developed to describe the photophysical properties and photochemistry precisely. In this lecture, we focus on the quantum chemical approaches for the excited states and their applications to various photochemical processes and photophysical properties.

In the first part of the lecture, quantum chemical methods for molecular excited states will be introduced with regard to their formulation, basic character and applicability. In the second part, we will focus on the recent SAC-CI and TD-DFT studies on the large conjugated systems with near infrared (NIR) absorption, the solvent effects using polarizable continuum model (PCM), and the charge transfer indexes for the excited states.

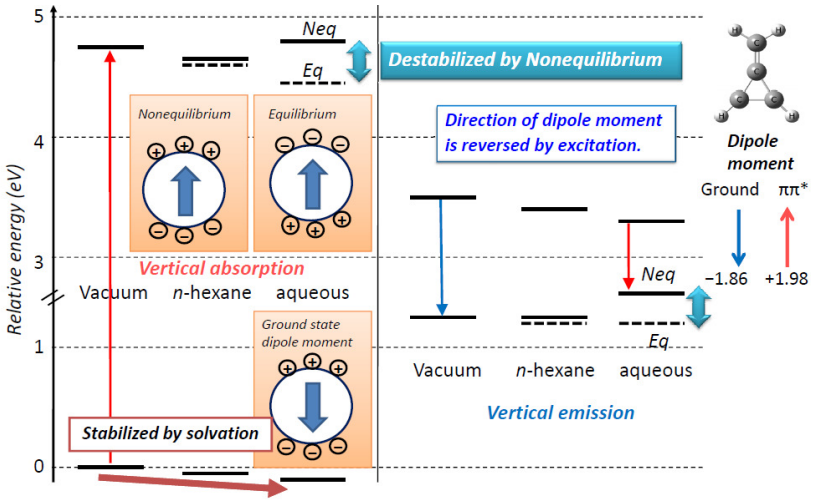

Figure 1. Solvent effects on excited states by non-equilibrium PCM-SAC-CI

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