My research field was reaction dynamics and quantum chemistry. We were interested in reactions in the excited state induced by photons. One example is retinal. Retinal is embedded in rhodopsin protein, which is responsible for vision of vertebrate animals including human. When the retinal is exposed to light, the 11-cis form is excited and isomerized to the all-trans one. This process has been investigated experimentally as well as theoretically. We carried out simulation of the photoisomerization of rhodopsin and isorhodopsin, which includes 9-cis retinal instead of 11-cis retinal. The simulation reproduced faster and more efficient isomerization in rhodopsin than in isorhodopsin. In the excited state, rhodopsin shows a straightforward dynamics, whereas isorhodopsin dynamics is rather complicated and in a back-and-forth manner. The latter complicated dynamics would be mainly due to a narrow space near the active dihedral angle =C8−C9=C10−C11= (ϕ9) created by Thr 118 and Tyr 268 in opsins as shown in Fig. 1. Rhodopsin gives bathorhodopsin only while isorhodopsin yields a byproduct. The rigorous selectivity in rhodopsin would be another reason why rhodopsin is selected biologically. Comparison with our previous opsin-free investigations reveals that opsin tends to confine the twist of the active dihedral to only one direction and funnels transitions into the vicinity of minimum energy conical intersections (MECI). The twist-confinement totally blocks simultaneous twisting of ϕ9 and ϕ11 (=C10−C11=C12−C13=) and enhances the quantum yields. The opposite rotation of ϕ9 and ϕ11 (“wring-a-wet-towel” motion) takes place upon photoexcitation, which also does without opsin. The wring-a-wet-towel motion is dynamically enhanced in comparison with the one expected from locations of the MECI.

My other recent topics were (1) ligand-exchange reactions in CooA, which is one of gas sensor protein (Fig. 2), (2) photochemical dynamics of indolylmaleimide derivatives.

References