Contribution of Computational Science and Simulation in Industrial Research, focusing on two recent activities: Photonic Molecular Design and NMR Chemical Shift by FMO method

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Theoretical study has been established as an indispensable area in chemical industries. During two recent decades, this is recorded in history. It is, however, only a limited partial potential in theoretical study that has so far realized. The purpose of the current presentation is to demonstrate that tremendous numbers of challenging subjects, for theory and simulation researchers, are still waiting to be analyzed in industries.

We show the various real subjects that we had committed and that theoretical study contributed to advance the industrial researches and developments. Examples include the molecular design of dyes and photo-responsive photonic materials, catalyst design, biological molecular design, and signal processing.

Special attention will be paid on the new two subjects. The first one is the photo-responsive molecule in which environmental field effect is crucial. It is closely related to the Tg properties of polymer. The second is a new methodological development of FMO based NMR chemical shift study, in an attempt to understand the drug and protein interaction.

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