

Hirofumi SATO



Associate Professor, Department of Molecular Engineering, Graduate School of Engineering, Kyoto University

【E-mail】 hirofumi@moleng.kyoto-u.ac.jp

【Speciality】 Theoretical Chemistry

【Keywords】 Statistical Mechanics for Molecular System, Hydrogen bonding Network

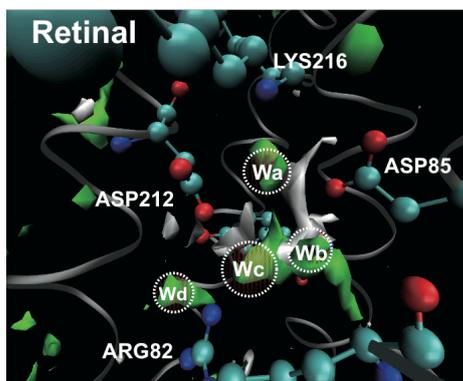
【Research Subject】

Theoretical Studies on proton and hydrogen bonding in biological molecules

Research Group Activity

Development and applications of statistical mechanical theory for molecular system

Development and applications of quantum chemical methods



$$A^-B^+ : \sum_{\mu \in A} \sum_{\nu \in A} \langle \phi_i | \chi_{\nu}^{\sigma_1^+} \chi_{\mu}^{\sigma_2^+} \varphi_{\nu}^{\sigma_2^-} \varphi_{\mu}^{\sigma_1^-} | \phi_i \rangle,$$

$$A - B : 2 \sum_{\mu \in A} \sum_{\nu \in B} \langle \phi_i | \chi_{\nu}^{\sigma_1^+} \chi_{\mu}^{\sigma_2^+} \varphi_{\nu}^{\sigma_2^-} \varphi_{\mu}^{\sigma_1^-} | \phi_i \rangle,$$

$$A^+B^- : \sum_{\mu \in B} \sum_{\nu \in B} \langle \phi_i | \chi_{\nu}^{\sigma_1^+} \chi_{\mu}^{\sigma_2^+} \varphi_{\nu}^{\sigma_2^-} \varphi_{\mu}^{\sigma_1^-} | \phi_i \rangle,$$

Development and applications of new theories for chemical processes in solution

Structure of ionic liquid (IL) and chemical reaction in IL.

