化学系セミナー（物理化学分野）のお知らせ

Dynamic Heterogeneity:
Origin, Analytical Prediction and Artifacts

講演者：　Professor Pratik Sen

（Department of Chemistry, Indian Institute of Technology Kanpur）

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連絡教員：化学系　腰原 伸也　(内線2449)

Seminar of Department of Chemistry, Tokyo Tech.

Dynamic Heterogeneity: Origin, Analytical Prediction and Artifacts

Professor Pratik Sen

Department of Chemistry, Indian Institute of Technology Kanpur, Kanpur – 208 016, India
E-mail: psen@iitk.ac.in

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Molecular level structure and dynamics decide the functionality of a solvent. One intriguing aspect of such structure and dynamics is heterogeneity. Generally, dynamic heterogeneity in a media is identified by recognizing the viscosity decoupling of the dynamics (i.e., $\tau_x \propto \left(\frac{\eta}{T}\right)^p$ with $p \neq 1$). In this seminar, a physical understanding of dynamic heterogeneity will be presented along with the experimental approaches to better correlate viscosity decoupled dynamics and dynamic heterogeneity.

A simple analytical model was constructed and validated to understand and predict viscosity decoupling and associated dynamic heterogeneity in a solvent. We assumed that SE relationship is locally satisfied, but their spatial average shows a breakdown. We showed that for a dynamically heterogenous media $\log(\tau_x) = \log\left(\frac{\eta_{bulk}}{T}\right) + \frac{E_\mu - E_{bulk}}{2.303\,RT} + \log C$, where the second term on the right-hand side leads to the viscosity decoupling. We further argued that a viscosity decoupling could be observed only if the sampling is done from the micro heterogeneous region. We identified that while dynamically heterogeneous media will show a breakdown from the Stokes-Einstein (SE) relationship ($p \neq 1$), the vice-versa is not automatically true. Therefore, one should be cautious in relating viscosity decoupling to dynamic heterogeneity. We developed two analytical method to determine dynamic heterogeneity from viscosity decoupling in a better way. First one is based on selective probing of differently diffusing sub-population and the second one is based on the photo-selection of different subpopulations in a heterogenous system.

References

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2) Nilimesh Das, Navin Subba and Pratik Sen *J. Photochem. Photobiol. A: Chem* **2022**, *436*, 114361.
3) Ejaj Tarif, Nilimesh Das and Pratik Sen *J. Phys. Chem. B* **2023**, *127*, 7162.
4) Nilimesh Das, Tanmoy Khan, Pratik Sen *Chem. Phys.* **2024**, *577*, 112138.