東京大学大学院工学系研究科エネルギー・資源フロンティアセンター
環境調和型エネルギー資源開発工学（JX 日鉱日石開発）寄付講座

Reservoir Engineering Research Institute & Peking University / Yale University

Abbas Firoozabadi教授 特別講演会

日　時：平成 29 年 11 月 9 日（木）13:20 ～ 14:50（受付開始 13:00）

場　所：東京大学工学部 3号館3階 33 号講義室
（東京都文京区本郷 7-3-1 本郷キャンパス）

“Molecular Structure in Hydrocarbons, Water/Brine, and Rock Substrates in Bulk and at Interfaces”

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Distinguished Visiting Professor
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Knowledge of molecular structure in bulk and at interfaces helps with efficient hydrocarbon energy production and stewardship of the environment. Natural gas, which is perhaps the premium fuel of the twenty first century can be produced from shale formations. There are many complexities in gas production from shale. There is no known method to measure the quantity of adsorbed gas when a shale rock is exposed to high pressure fluids. The water in deep subsurface formations contains large quantities of salts. When functional molecules are added to water to change properties, salt affects the solubility through different structures. Sometimes knowledge of mechanisms due to different effects become vague. Production of hydrocarbons from deep water has complexities and risks and environmental effects which can be addresses by use of small quantities of functional molecules. Molecular engineering can alleviate many transport problems.

This presentation will cover three examples from our recent work. We will first discuss sorption in shale media and demonstrate that the integration of measurements and molecular modeling should be combined to determine adsorption. Next we will discuss hydrophobicity and the effect of NaCl salt in methane hydrates. The effect on functional molecules both in the bulk and on the surface will be covered. The third topic relates to interfacial charge in water-normal alkanes to shed light on measured zeta potentials and the effect of pH on interfacial tension. We will use measurements and molecular dynamics simulations including steered molecular simulations and umbrella sampling to gain insight into various mechanisms and processes.

コーディネーター：佐藤 光三 (FRCER センター長、教授) & 小林 肇 (システム創成、FRCER 連携研究員、准教授)

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