

# YNU グリーンマテリアルイノベーション(GMI)研究拠点講演会／触媒学会規則性多孔体勉強会のご案内

## “Toward Rational Synthesis of Novel Zeolites for Applications as Catalytic and Energy Materials”

講師：Dr. Dan Xie (Chevron, USA)



日時： 2018年8月10日(金)16:15～17:45  
場所： 横浜国立大学 化学棟 211 セミナー室

アメリカの石油スーパーメジャーであるシェブロン(Chevron)社で規則性多孔体材料の構造解明に関する基礎研究を精力的に行っている Dr. Dan Xie が来日される機会に、触媒学会規則性多孔体研究会との共催で、横浜国大にて講演会を開催することになりました。新規ゼオライトの合理的な創製へ向けて、車の両輪ともいえる「合成」と「構造解析」の新しい概念について基礎事項を含めてご講演いただきます。物質の化学変換(ものづくり)やエネルギー分野とも密接に関連します。フランクな意見交換を行いますので、皆様のご参加を歓迎いたします。

### Abstract:

Zeolites play important roles in the fields of catalysis, adsorption-separation, and ion exchange. Such industrially important applications have promoted researchers to continue discover zeolites with new structures and broader composition range. Traditionally, novel zeolites are discovered in a trial-and-error manner, and it is not easy to predict which specific zeolite is going to be formed using which specific organic structure-directing agents (SDAs). Although the zeolite crystallization mechanism is still not well understood, it is known that both thermodynamics and kinetics control the crystallization process and the product selectivity, and the kinetics seems to be a more dominant factor in majority of cases. While the kinetics is difficult to predict or model, recent developments on modeling thermodynamic interaction between zeolite framework and organic SDA did increase the success rate for rational synthesis.

In this presentation, some basics on zeolite material and its application will be introduced, followed by a brief discussion of cutting-edge techniques for its complex structure elucidation. In the last session, I will demonstrate how we can utilize structural analysis techniques together with molecular modeling to guide new zeolite discovery.

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## 講師紹介 (Short Biography):

Dr. Dan Xie is currently a Senior Research Scientist at Chevron Energy Technology Company. He also serves as a member of the Structure Commission at the International Zeolite Association (IZA) and lectures the graduate students at the Chemical Engineering Department at UC Berkeley.

He received his Ph.D. degree in crystallography from ETH Zurich in 2010, where he was awarded the ETH Medal for his thesis work on methodology development of polycrystalline structure determination.

He joined Chevron in 2011 and began a program in searching for new zeolite catalysts with a strong emphasis on integrating molecular modeling and structural analysis to aid in the synthesis. Dr. Xie is a co-author and co-inventor on more than 40 scientific publications and 50 technology patent applications, some of his discoveries have been successfully commercialized and applied in specific industrial processes.