

演題：**Revisiting the paradigm of transition states
and reaction mechanisms**

講師：**Prof. Srihari Keshavamurthy**
(Indian Institute of Technology
Kanpur, India)



日時：2019年6月24日(月)14:30～15:30

場所：理学部本館 N-308 室

要旨：The concepts of transition states and reaction mechanisms have been around for more than a century. Indeed, these concepts have shaped modern chemistry as we know it and it is hard to think of understanding chemical reactivity without them. In fact, we have gotten so comfortable with these models that we believe every reaction must conform to 'the paradigm'. However, over the last two decades, thanks to developments in experiments and theory, uncomfortable questions are being asked about the usual assumptions that one makes to deduce the reaction mechanisms. Are these examples just exceptions? Can we still fit these new observations by making small extensions to the old paradigm? Or, do we have to shift paradigms altogether?

In this talk I will briefly introduce and discuss some of these recent developments and the challenges that they pose to theoretical chemists.

本講演は、大学院総合化学院『化学研究先端講義（修士課程選択科目）／総合化学特別研究第二（博士後期課程選択科目）』の一部として認定されています。

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