

マテリアルサイエンス系セミナー(第8回)

テーマ Control over Molecular Photoactivity in Porous Materials :Insights from Multiscale Simulations

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場所: マテリアルサイエンス系研究棟4棟8階 中セミナー室

講演要旨:

Synthetic control over the properties of porous materials, including zeolites and covalent organic frameworks (COFs), has enabled the creation of nanoscale environments that can enhance or suppress molecular function. A core focus of our research program is the development of multiscale simulations to understand the effects of encapsulation and embedding of photoactive molecules in porous materials. In this presentation, we first examine the electronic consequences of embedding acenes of varying length in a 2D COF with a focus on whether such materials can meet energy level criteria for singlet fission, the generation of two triplet excitons from a single photoexcitation. DFT-based molecular dynamics sampling of electronic energy levels and couplings reveals considerable fluctuations in the embedded acenes' relative orientations at room temperature and confirms strong sensitivity of the electron mobility to these orientations. A materials informatics approach is then introduced to explore alternative architectures more amenable to singlet fission. Through the construction of contact profiles for a library of acene linker derivatives, we can identify chromophores that adopt more favorable orientations for singlet fission. We argue that 2D COFs represent a third architectural paradigm, complementary to organic molecular crystals and solvated organic dimers, in the search for efficient singlet fission materials. Time permitting, we will discuss related simulations examining the effects of encapsulation in a porous aluminosilicate on the charge-transfer state lifetime of a popular photoredox catalyst.

講演者略歴:

Tim Kowalczyk is a computational materials scientist and an Assistant Professor at Western Washington University with joint appointments in Chemistry, Materials Science, and Energy Studies. Dr. Kowalczyk earned a B.S. in chemistry and mathematics from the University of Southern California and a Ph.D. in physical chemistry from MIT. Following a JSPS Postdoctoral Fellowship at Nagoya University, in 2014 he joined the faculty of WWU, where he is currently the Snohomish PUD Professor of Energy Studies.

参加申込・予約は不要です。直接会場にお越しください。
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