量子物理学・ナノサイエンス第 266 回セミナー

Computational studies of photoelectrocatalytic systems

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概　要

Recent progresses in theory of catalytic reactions led to successful computationally guided discoveries of novel catalyst systems. However, simultaneously, it also disclosed presence of intimate relation between energetics and kinetic of elemental catalytic reaction processes for multi-step catalytic reactions such as oxygen evolution, CO_2 reduction, ammonia synthesis, a part of which has been known as Evans-Polanyi relation. Presence of such a relation suggests that catalytic system consisting of a homogeneous and a single component catalyst material will likely to face a great challenge in improving catalytic performance compared to known conventional catalysts since substituting the catalyst material in hope of improving kinetics of rate limiting step will likely to lead to a worse kinetics of the other steps, one of which may turn into the rate limiting step. This relation also poses a challenge in controlling selectivity since the kinetics of branching reactions are also likely to be correlated in a linear fashion. At the presentation, we will first discuss about underlying concepts based on our research experiences about computational design of novel catalyst [1,2] as well as about transport properties of reaction intermediate at solid-liquid interfaces [3]. We will then discuss about the factors that need to be further studied in order to overcome the currently known challenges such as the discrepancy in timescales between photochargecarrier generation and catalytic reaction, the problem posed by the scaling relation, etc.

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1. W. I. Choi *et al*. J. Phys. Chem. C **117**, 21772 (2013)
2. W. I. Choi *et al*. Adv. Energy. Mater **5**, 1501423 (2015)
3. B. C. Wood *et al*. J. Am. Chem. Soc. **135**, 15774 (2013)

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