グローバル COE 物質科学イノベーション講演会

演 題： **Chemical Reactions in Virtual Laboratory**

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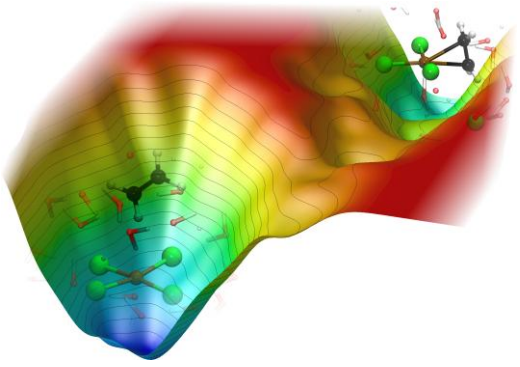
日 時： 2012 年 3 月 7 日（水）15 : 00 ～ 16 : 30

場 所： 理学部 7 号館 2 階 7-2-19 室

要 旨： *In silico* study of complex chemical reactions in condensed matter systems and thereby accessing molecular level details of reaction mechanisms and associated free energies remains as a great challenge in the field of molecular simulation. Employing the latest developments of *ab initio* molecular dynamics techniques and the state-of-the-art computer technology, we are able to tackle the time-scale and the length-scale bottlenecks in computer simulations. These enable us to address some of the challenging problems in chemistry and biology. Some examples will be presented where large scale simulations have unraveled the detailed mechanisms of enzymatic reactions, homogeneous catalytic reactions in aqueous solutions and heterogeneous catalytic reactions. Finally, I will be addressing some of the current challenges in the field of *ab initio* molecular dynamics.



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