２１世紀 COE　公開講演会

日時　2004 年 6 月 2 日 14 時 30 分～16 時 00 分

場所　化学教室本館４階講義室

講師　**Dr. Gopinathal Sankar**

(Davy Faraday Research Laboratory

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演題　**“Structure of active sites in Redox molecular sieves”**

サンカー博士は英国王立研究所の上級研究員として，ジョン　トーマス教授らと X 線吸収分光法を用いたゼオライトなどの構造解析を精力的に行っている新進気鋭の研究者です。同博士は英国 Daresbury 放射光施設のメインユーザーとして，最近，X 線回折とＸＡＦＳを組み合わせた手法を展開していますが，今回の来日の機会に，最近の研究成果について講演していただく予定です。

当日は１４時３０分まで先端化学集中講義がありますが，その直後から始めますので，多数の参加を期待しています。

担当　太田　俊明　（２４３３１）

STRUCTURE OF ACTIVE SITES IN REDOX MOLECULAR SIEVES

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It is well known that well-defined crystalline microporous materials offer the most effective shape-selective catalytic reactions. Invariably the catalysis is mediated by the presence of a hetero-atom that substitutes in the framework, replacing the main constituent such as Si(IV) in silicate based systems, Al(III) or P(V) in aluminophosphates systems. Although the structure of these solids determined by the most powerful tool, X-ray diffraction, it is often very difficult to pin down the structure of the hetero-atom, since their concentrations are invariably low and more importantly they are substituted in random, which prevent the determination of their 'local' structure accurately. Although X-ray absorption spectroscopy, in particular EXAFS, provides one-dimensional information, it has been found that this technique is best suited for the determination of the structure of the hetero-atom. While combining these two techniques, XRD and XAS is powerful in these types of solids, introducing in situ methods have made this even more powerful in determining the structure of microporous materials and relate them to catalytic properties. Examples from Ti(IV) substituted silicate system, Fe(III) or Co(II) substituted aluminophosphates will be presented to demonstrate the power of XANES, EXAFS and XRD measurements. The importance of the use of multiple-scattering procedures in the determination of local-structure will be shown and in addition, the advantage using combined XRD/XAS refinement method will be demonstrated.