平成１９年度　第３回VBL講演会

日時：　２月１２日（火）　　１６：３０～１７：００

場所：　工学部　大会議室

講師：　Jianguo Wang 教授（Director of State Key Lab. of Coal Conversion, Deputy director of Institute of Coal Chemistry, Chinese Academy of Sciences）

題目：　Experimental and Theoretical investigation into the structure, acidity and catalysis of Zeolites

【講演概要】

Beginning with a brief introduction to R&D activities on clean coal technology in State Key Laboratory (SKLCC) and Institute of Coal Chemistry (ICC) under Chinese Academy of Sciences (CAS), this presentation will focus on the structure, acidity and catalysis aspects of zeolites. The sitting of heteroatom such as B, Fe, Ga, and Al substituted to Si in zeolites is determined and the acidity of the substituted zeolites is investigated by Density Functional Theory method. To get insight into the nature of shape selectivity of zeolites, a Monte Carlo model is developed and the adsorption, diffusion and reaction in zeolites are simulated.