

造系统重构, 最终实现手性化学品的高效绿色生物制造。

关键词: 生物制造 手性化学品 理性设计 性能强化 系统重构 绿色制造 高效

Project Report of Bio-manufacturing of Chiral Chemicals

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Abstract: Bio-manufacturing of chiral chemicals uses the cross means of biology, chemistry, engineering and informatics. It focuses on the high quality synthesis of optical pure chemicals, in a quick, efficient, high selective and green way. Based on the analysis of protein structure, molecular biology, synthetic biology, chemical synthesis, reaction engineering and system engineering, it provides creative design thinkings and new scientific methods for the clean, efficient, economic and fast production of chiral chemicals. Through rational design, reaction performance enhancement and reconstruction of manufacturing systems, the efficiency green-manufacturing of chiral chemicals will be realized.

Key Words: Bio-manufacturing; Chiral chemicals; Rational design; Performance enhancement; System reconstruction; Green-manufacturing; High efficiency

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手性砌块库和合成模块库的构建

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摘要: 成功构建了包括新型卤代醇、羟基氟、芳香醇、脂肪醇和芳香胺的手性砌块库, 涵盖108种手性化合物。构建了5种新型酶-化学手性反应模块, 例如脂肪酶拆分-Pd/LDH-DS消旋反应模块能够在常温下拆分芳香胺类, 其中底物转化率99%, 产物ee值99%, 突破生物拆分过程理论转化率仅为50%的不足, 过程的原子经济性与转化效率较高, 具有较大的创新性。

关键词: 手性砌块 合成模块 库 化学-酶法 脂肪酶 拆分

Construction of Chiral Block Library and Synthesis Module Library

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Abstract: A chiral block library, including 108 kinds of chiral chemicals, were constructed. 5 types of novel chem-enzymatic synthesis modules were also developed. For example, the module of lipase coupled with Pd/LDH-DS was successfully used in the resolution of aromatic amine with the excellent results of conversion of 99% and eep of 99%. The atom economy and conversion efficiency were greatly improved with this novel module.

Key Words: Chiral block; Synthesis module; Library; Chem-enzymatic method; Lipase; resolution

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构造热演化与页岩气的改造和保存研究

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摘要: 该文重点开展了中国南方典型盆地构造热演化特征及页岩气形成的地质背景的研究, 初步开展了构造改造对页岩储层物性和页岩气赋存形式的影响的研究。所取得的主要进展有: (1) 以全面调研及大量野外地质调查为基础, 结合地球物理资料解释与分析, 多尺度详细剖析下扬子地区的构造特征, 盆地演化及其对关键暗色页岩分布与保存的影响, 揭示江阴-无锡滑脱褶皱带为相对稳定区块; (2) 以野外地质调查、样品采集及室内扫描电镜观测为基础, 结合挤压构造活动数值模拟, 探索了构造改造对下扬子页岩储集空间的影响, 揭示了强烈的挤压、剪切会严重破坏页岩中的孔洞结构, 但断层活动影响的范围有限, 褶皱冲断带内

的宽缓向斜页岩气保存条件较好；(3)Ro以及新获得的低温热年代学测试数据研究结果表明四川盆地热历史可大致以260 Ma为界分为P2末期之前的热流升高阶段和之后的热流降低阶段及随后的低热流发展阶段，晚二叠世峨眉山地幔柱和中晚三叠世以来前陆盆地演化是四川盆地热演化主要影响因素。

关键词：下扬子地区 四川盆地 构造演化 构造变形样式 页岩气保存

Progress Report of Tectono-thermal Evolution and Alternation and Preservation of Shale Gas

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Abstract: For the first two years, our research focused on the Tectono-thermal evolution and shale gas formation geological background of typical basins in southern China. And we have started to investigate the influences of structural alternation on the shale reservoir and shale gas occurrence. 10 faculties and 12 graduate students worked in this project. More than 2000 papers of geological background have been collected. 653 samples from 128 observation sites were collected during the past 7 field works. And we have mapped 10 geological cross sections and accomplished more than 700 experimental tests. The major progresses so far include: 1)Based on the analysis of field observation,drilling data and geophysical data,we interpreted the structural deformation characteristics and basin evolution of Lower Yangtze region and its influence on the distribution and preservation potential of the key shale layers. We suggest that the detachment-fold belt of Jiangyin-Wuxi is relative structural stable belt in the Lower Yangtze region; 2)Based on the field observation, sample collection and SEM analysis, and DEM modeling of compressional structural deformation, we investigated the influence of structural alternation on the reservoir properties of the Lower Yangtze shale, and concluded that strong compression and shear deformation do great damage to the pore structure of the shale, but the damage resulted from faulting is limited to the zone close to the fault, the broad synclines within the fold-and-thrust belts still have good shale gas preservation potential; 3)Based on Ro and low temperature thermochronology data, we divided the thermal history of Sichuan basin into two stages, the heat flux increasing and decreasing stages before and after later permian respectively. Emeishan mantle plume in the later permian and the tectono-thermal evolution of foreland basin since mid-later triassic are the controlling factors for the thermal evolution of the Sichuan basin.

Key Words: Lower Yangtze region;Sichuan basin;Tectonic revolution;Structural deformation styles;Shale gas preservation

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糖类衍生物催化制液体烷烃燃料的基础研究

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摘要: 该研究针对第三个关键科学问题“解聚产物催化转化制备先进液体燃料的机理及产物选择性控制规律”开展基础性研究工作。在糖类衍生物水相催化制液体烷烃燃料的反应机理、产物控制规律研究和相关高效催化剂体系设计等方面进行了探索。针对糖类衍生物水相催化合成HMF,发展了高效的类微乳反应体系和NaHSO₄-ZnSO₄催化剂体系,可有效避免副产物生成和HMF的进一步降解,获得高达57%的HMF收率。发展MOFs内嵌杂多酸和Ru粒子的高效催化剂,通过金属与酸的功能匹配,实现了纤维素等一步转化为山梨醇,山梨醇收率达到58%。制备了Ni基金属-酸双功能催化剂应用于山梨醇/木糖醇转化为C5/C6烷烃,通过金属组分、载体等的调控作用和反应机理研究,实现C5/C6烷烃产物的定向催化合成,收率超过90%。针对糠醛与丙酮的缩合反应,设计合成了高效MgO/NaY固体碱催化剂,碱性质及MgO与NaY的协同催化作用可有效活化糠醛与丙酮分子,加快反应速率,获得高达98%的C8-C15缩合产物,设计合成了Pt/SiO₂-ZrO₂催化剂,通过调控催化剂的组成结构和产物加氢脱氧路径分析,获得收率达到70%的C8-C15烷烃产物,催化剂连续运行120 h不失活,具有较好的稳定性。针对酚类衍生物催化制备液体烷烃燃料,设计合成了离子液共聚物负载的Ru催化剂,通过离子液共聚物稳定Ru纳米粒子的金属-酸双功能的协同催化作用(金属中心的C-C键加氢饱和,酸中心的C-O断裂),实现了苯酚及其衍生加氢脱氧高效转化为液体烷烃。针对苯酚选择性加氢制环己酮,设计合成了高效的聚苯胺修饰碳纳米管负载Pd催化剂,通过聚苯胺修饰碳纳米管的电子调控对苯酚及其衍生物的选择性吸附和Pd活性组分的协同加氢作用,实现了苯酚及其衍生物定向转化为环己酮衍生物,环己酮收率高达99%。在上述研究基础上,我们率先在国内建立了年产150吨规模的生物汽油验证研究系统。

关键词：糖 水相催化 液体烷烃 基础研究

Basic Research on Liquid Alkanes From Sugar Derivatives by Aqueous Phase Catalysis

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