

## Bao Xinhe, Dalian Institute of Chemical Physics, Chinese Academy of Sciences

Prof. Xinhe Bao's research focuses mainly on the fundamental understanding of catalysis, and its application to the development of new catalysts and catalytic processes for energy conversion, especially in the fields of clean coal and natural gas utilization. Prof. Bao developed the concept of synergetic confinement effect for catalysis within carbon nanotubes. Based on this concept, Prof. Bao and his team created highly efficient catalysts for coal conversion to  $C_2$  oxygenates and olefins via syngas. Prof. Bao and coworkers also developed the concept and the theoretical model of interface confinement to describe the strong interaction between oxide nanostructures and noble metals surfaces. On this basis, they prepared highly efficient catalysts for the selective oxidation of CO, which is the key to remove the trace amount of CO poison from hydrogen under the realistic operating conditions of fuel cells. Recently, Prof. Bao and his team developed the concept of lattice confinement to introduce iron active centers within a silicate matrix, and created a highly efficient single-site iron catalyst for the direct and non-oxidative conversion of methane into major chemical feedstock, such as ethylene, benzene, and hydrogen. His research has brought major impact in both the international academic community and industries.

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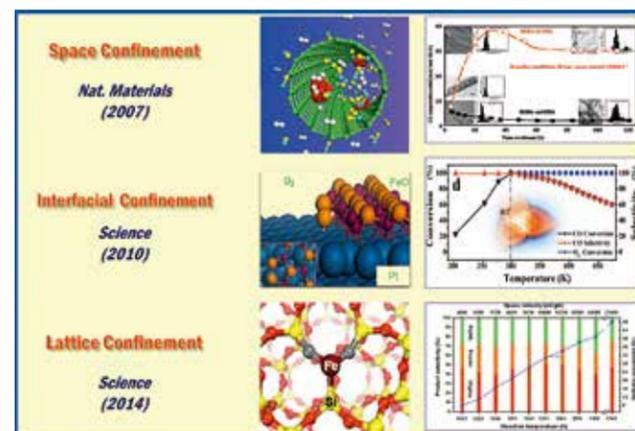
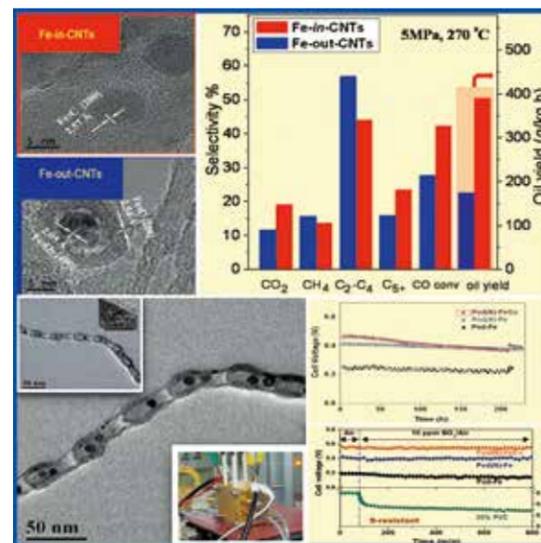
获奖个人所在单位：中国科学院大连化学物理研究所

## 主要科技贡献：

包信和院士长期从事物理化学研究，在催化基础理论研究和化石能源高效转化过程新型催化剂研制和开发等方面做出了出色的研究成果。发展出碳纳米管对金属和氧化物纳米粒子的电子调制作用的“协同限域”概念，创制了合成气高效转化催化剂，在煤经合成气制取  $C_2$  含氧化合物和低碳烯烃过程中显示了独特的催化性能；发展出金属氧化物纳米结构与贵金属表面强相互作用的“界面限域”模型，制备出高性能的一氧化碳选择氧化催化剂，成功应用于燃料电池实际操作条件下的燃料氢气中微量 CO 的高效脱除；首创硅化物晶格限域的单中心铁催化剂的“晶格限域”催化的概念，构建了单中心铁催化剂，实现了甲烷在无氧条件下选择活化，一步高效生产乙烯，芳烃和氢气等高值化学品，在国际学术界和产业界形成了重要影响。

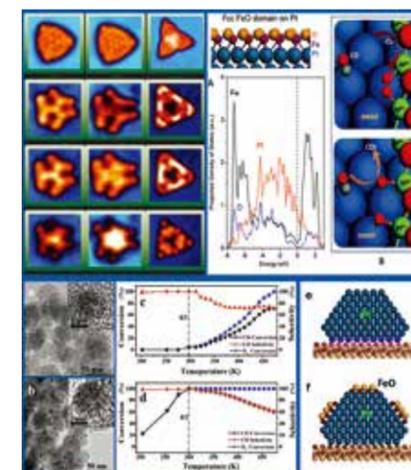
碳纳米管的“协同限域效应”：纳米级管腔为催化提供了独特的限域环境，促进了 Fe 催化剂在费托反应条件下生成更多的活性碳化物，从而显著增强其费托反应性能。封装于碳纳米管的非贵金属铁作为质子膜燃料电池阴极催化剂催化氧化还原反应中显示优异的活性和稳定

The “synergetic confinement effects of CNTs” in catalysis: The nanochannels of CNTs provide an intriguing confined environment for catalysis where Fischer-Tropsch Synthesis activity was observed because of facilitated formation of iron carbide species inside CNTs under reaction conditions. A non-precious metal Fe catalyst encapsulated within CNTs with a chainmail structure exhibits not only a high activity but also high stability as a cathode catalyst for Oxygen Reduction Reaction (ORR) in Proton Exchange Membrane Fuel Cell (PEMFC)



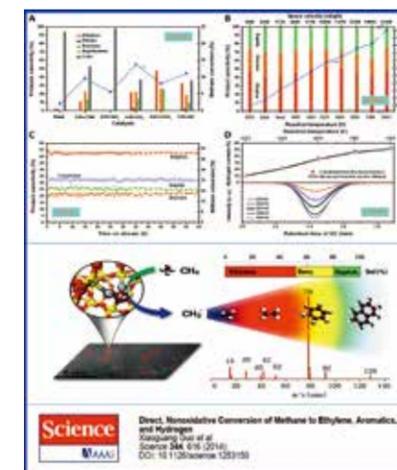
包信和院士及其团队经过多年研究提出和发展的“催化中限域效应”概念，包括“碳纳米管的协同限域效应”、“界面限域效应”和“晶格限域效应”。这些概念已经用于指导重要能源转化过程高效催化剂的设计制备，包括煤经合成气制乙醇，燃料电池 CO 选择氧化，甲烷直接转化制乙烯和芳烃

The concept of the confinement effects in catalysis, which Prof. Bao and his team put forward and developed over years, including Synergetic confinement effects of CNTs, Interface confinement and Lattice confinement effect. These concepts, have guided design of catalysts for several important processes in the field of energy, such as coal conversion to ethanol via syngas, selective removal of CO from excess  $H_2$  for fuel cell applications, and direct conversion of methane to ethylene and aromatics



包信和院士及其团队发现了氧化物纳米结构与贵金属界面的强相互作用，从而使活性氧化物纳米结构在特定的催化反应中显示出独特的稳定性，这一发现为贵金属催化剂的替代研究提供了新的途径

Prof. Bao and his team proposed the concept and the theoretical model of 2D interface confinement to describe the strong interaction between oxide nanostructures and noble metals surfaces. Their research shows that active oxide nanostructures of transition metals can be stabilized on noble metal surfaces and exhibit excellent catalytic performances, implying possibility of reducing the usage, or even replacement of noble metals



晶格限域的单铁中心催化甲烷无氧直接转化制乙烯和芳烃新过程：反应温度为 109°C 时，甲烷单程转化率为 48%，产物乙烯和芳烃的选择性大于 99%。该过程与传统天然气利用途径相比，摒弃了高能耗的气化单元，而且反应本身无二氧化碳排放，为未来天然气和页岩气的高效利用提供了一条新途径

An atom-economical process converting  $CH_4$  directly to ethylene and aromatics is enabled by a catalyst with lattice-confined single iron sites embedded within a silicide matrix. The reaction at 1090 °C delivers a methane conversion of 48% and the total selectivity to ethylene and aromatics at above 99% with no  $CO_2$  emission. This process reduces the operation units by skipping the energy-intensive syngas production unit and the reaction itself gives no  $CO_2$  emission, and provide a new approach for efficient utilization of natural gas and shale gas