中国科学院大连化学物理研究所
优秀博士后奖励基金申请表

申 请 人： KAMRAN QADIR

研 究 组： 501组

学科专业： 物理化学

合作导师： 申文杰

填表日期： 2016年4月16日

中国科学院大连化学物理研究所制

<table>
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<tr><td>学历/学位</td><td>博士研究生</td><td>专业技术职务</td><td></td></tr>
<tr><td>毕业院校</td><td>Korea Advanced Institute of Science and Technology (KAIST)</td><td>专　　业</td><td>物理化学</td></tr>
<tr><td>（拟）入站时间</td><td>2016-4-16</td><td>入站性质</td><td>☑统招统分　　☐在职人员</td></tr>
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<tr><td rowspan="4">学习简历</td><td>起止年月</td><td>所在单位/专业</td><td>所获学位</td></tr>
<tr><td>2011-9-1 至 2015-8-30</td><td>Korea Adv. Inst. of Sci. & Tech. (KAIST), Republic of Korea</td><td>博士</td></tr>
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<tr><td rowspan="2">工作经历</td><td>起止年月</td><td>所在单位</td><td>职务</td></tr>
<tr><td>2015 年 4 月至今</td><td>中国科学院大连化学物理研究所</td><td>博士后</td></tr>
<tr><td rowspan="3">博士学位论文摘要</td><td>博士论文题目</td><td colspan="2">Uncovering the Role of Surface Oxide and Metal-oxide Interface in Engineering Active Metal Nanocatalysts under Gas Phase Catalytic Reaction</td></tr>
<tr><td>指导教师姓名</td><td colspan="2">Professor Jeong Young Park</td></tr>
<tr><td colspan="3">We studied Ru nanoparticles using Ambient Pressure X-ray Photoelectron spectroscopy (AP-XPS) to investigate catalytically active species on Ru nanoparticles under reaction conditions. We found that the smaller Ru nanoparticles form bulk RuO_2 on their surfaces, causing lower catalytic activity. As the size increases, the core−shell type RuO_2 becomes stable. We studied the nature of Ru oxides on a Ru polycrystalline film under reaction conditions. Our reaction studies showed substantial deactivation of the Ru film during catalytic CO oxidation. This is correlated with irreversibly formed bulk Ru oxide, as shown by AP-XPS. We also investigated two-dimensional Pt nanoparticle/titania catalytic systems under the CO oxidation reaction. Our results show an enhanced activity of Pt nanoparticles when the nanoparticle/titania interfaces are exposed. APD Pt shows superior catalytic activity due to the catalytically active nature of the mild surface oxidation and the active Pt metal and thus can be used for large-scale synthesis of active metal nanocatalysts. In the last study, we showed that engineering Metal-oxide interfaces in TiO_2-nanoporous (np) Au inverse catalyst results in enhancement of H_2 oxidation activity. We correlate change in activity with the active sites at perimeter interface between the TiO_2 and np-Au.</td></tr>
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入站前期科研情况简介

1、主持或参与项目情况：

序号	项目名称	项目来源	项目金额	起止年度	角色
1	Probing and control of metal nanoparticle and oxide interface	National Research Foundation of Korea	100,000,000 韩元	2011年5月1日至 2012年4月30日	参与
2	Sustainable energy engineering Technology (WCU)	National Research Foundation of Korea	690,000,000 韩元	2009年8月20日至 2013年8月31日	参与
3	Chemical reactions on the surface of Nanomaterials	Institute for Basic Science	3,558,926,000 韩元	2013年9月1日至 2015年12月31日	参与

2、论文发表情况：

序号	论文题目	期刊名	影响因子	发表年度/卷期/页码	排序
1	Pt/oxide nanocatalysts synthesized via the ultrasonic spray pyrolysis process: engineering metal–oxide interfaces for enhanced catalytic activity	Research on Chemical Intermediates	1.22	42, 211-222 (2016)	3
2	Tailoring metal-oxide interfaces of oxide-encapsulated Pt/silica hybrid nanocatalysts with enhanced thermal stability	Catalysis Today	3.89	265, 245-253 (2016)	4
3	Tailoring Metal-Oxide Interfaces of Inverse Catalysts of TiO2/Nanoporous-Au under Hydrogen Oxidation	Chemical Communications	6.834	51, 9620-9623 (2015)	**1**

	4	Catalytic Activity of Pt/SiO2 Nanocatalysts Synthesized via Ultrasonic Spray Pyrolysis Process under CO Oxidation	Applied Catalysis B: Environmental	7.435	154, 171-176 (2014)	3
	5	Nature of Rh Oxide on Rh Nanoparticles and Its Effect on the Catalytic Activity of CO Oxidation	Catalysis Letters	2.37	143, 1153-1161 (2013)	2
	6	Deactivation of Ru Catalysts under Catalytic CO Oxidation by Formation of Bulk Ru Oxide Probed with Ambient Pressure XPS	The Journal of Physical Chemistry C	4.772	117, 13108 (2013)	**1**
	7	Support Effect of Arc Plasma Deposited Pt Nanoparticles/TiO2 Substrate on Catalytic Activity of CO Oxidation	The Journal of Physical Chemistry C	4.772	116, 24054–24059 (2012)	**1**
	8	Intrinsic Relation between Catalytic Activity of Oxidation on Ru Nanoparticles and Ru Oxides Uncovered with Ambient Pressure XPS	**Nano Letters**	**13.592**	12, 5761–5768 (2012)	**1**
	9	Large Scale Synthesis and CO oxidation Study of FeCr Alloy Supported Pt Nanocatalysts by Electrical Wire Explosion Process	Catalysis Letters	2.37	142, 326 (2012).	8
	10	Trend of Catalytic Activity of CO Oxidation on Rh and Ru Nanoparticles; Role of Surface Oxide	Catalysis Today	3.89	185, 131-137 (2012)	2

11	Ultrathin Titania Coating for High-temperature Stable SiO2/Pt Nanocatalysts	Chemical Communications	6.834	47, 8412 (2011)	4
12	Current Trends of Surface Science and Catalysis Chapter 7	Springer-Verlag New York		2014	2

3、专利情况：

序号	专利名称	授权/申请	授权/申请号	起始日期	排序
1	아크 플라즈마 증착법을 이용한나노촉매제조방법 (Method for preparing nanocatalysts using arc plasma deposition Method）	授权	10-1472985	2014 年 12 月 9 日	3

4、获奖情况：

序号	奖励名称	奖励等级	授奖单位	奖励年度	排序
1	Best Poster Award		ENGE International Conference. Korean Institute of Metals and Materials	2014	1
2	Best Poster Award		Korean Vacuum Society	2012	1
3	First Prize Final Year Undergraduate Research Project Competition		GIK Institute	2009	1
4	Roll of Honor for High Distinction (3.77/4.00 SGPA)		GIK Institute	2009	1
5	Roll of Honor for Highest Distinction (3.94/4.00 SGPA)		GIK Institute	2008	1

博士后研究题目：Intrinsic Correlation between Atomically Engineered Metal-Oxide Interface and Catalytic Activity in Cu/Metal-Oxide/Alumina Nanocatalysts for TunableTechnological Catalysts

博士后工作的研究计划	（简述研究计划的可行性、先进性和创新性，理论和现实意义） **1. Research Programme** Overview of the proposed research program and plan is explained as follows: **1.1** Fabrication of atomically engineered Metal-Oxide interface(s) in nano-catalytic metal nanoparticles on oxide systems of ZnO, Ga2O3 and In2O3 of rod and sheet morphology The first critical step is to design well-controlled Metal-Oxide interface in metal/oxide based nanocatalysts. The underlying aim is to be able to probe intrinsic contribution of the metal-oxide interface(s) to the catalytic activity under gaseous reaction conditions. This will be achieved through synthesizing smart nano-structures (e.g. metal nanoparticles (NPs) of well defined sizes and Oxide nanostructures of atomically controlled nano-dimensions such as rod and sheet morphology of uniform size and shape), together with excellent dispersions of the individual components. The first system of interest that will be designed and tested for catalytic reaction studies is Cu/ZnO based nanocatalysts. Cu NPs of three different uniform sizes (1-2nm, 4-6 nm and 8-10 nm) will be deposited on 'Rod' and 'Sheet' morphology based Zinc oxide ultra-small nano-structures of uniform sizes and shape. In a similar fashion, we will synthesize Ga2O3 and In2O3 based nanocatalysts. **1.2** Visualizing enhanced Metal-Oxide interactions via advanced In-situ techniques and instrumentation to uncover atomic scale variations at active sites in working nano-catalysts under gaseous/reaction atmospheres In order to probe the intrinsic correlation between catalytic activity and the tailored metal nanoparticle-oxide nanostructure interface, it is critical to probe the active sites at interface perimeter during working conditions of the nanocatalysts. This will yield crucial insights into the atomic scale working of the catalyst to be directly applied to industrial catalysts and bridge 'Pressure Gap' across the lab-scale reaction conditions and technologically relevant highpressure conditions. For this goal, we will conduct in-*situ* probing of the interface via novel instrumentation including ambient pressure STM (Scanning Tunneling Microscopy) and 'Environmental TEM (Transmission Electron Microscopy)'. These techniques allow us to observe the structural changes occurring on the surfaces of the working nano-catalysts in real time under gaseous environments. It is expected that the adsorption/desorption of the reaction and products species respectively at active sites will be accompanied by atomic level structural changes on the active sites at Metal NPs-Oxide perimeter interface. Initial optimization of the nano-architectures of ZnO, Ga2O3 and In2O3 will be carried out using SEM/HR-SEM (Scanning electron microscopy) and TEM/HR-TEM. In additional, thorough structure of the nano-catalyst and its surface/bulk chemistry will be complemented by XRD (X-Rays diffraction) and XPS (XRay photoelectron spectroscopy). We will also carry out relevant surface area experiments such as metal dispersion measurement etc. using pulse chemisorption of CO/H_2.

博士后工作的研究计划

1.3 Catalytic Activity of the engineered nanocatalysts under reaction conditions to establish intrinsic correlation between active sites under reaction conditions and metal-oxide interface perimeter area

In the final step of the project, all 'Metal-Oxide' engineered nano-catalysts will be used to carry out catalytic reaction such as CO oxidation reaction. Carbon monoxide (CO) is one of the most-studied molecules among the many modern industrial chemical reactions available. Turnover frequency (TOF) in terms of oxidized CO molecules/active site will be calculated for each nano-catalytic system. Together with comparison with similar catalytic systems reported so far and after calculation of metal-Oxide interface perimeter area, a correlation will be established between metal-Oxide interface and catalytic activity. Stand-alone reference catalysts such as Cu nanoparticles on inert SiO2 support and Cu single crystals will be utilized for comparison with our nano-catalytic systems.

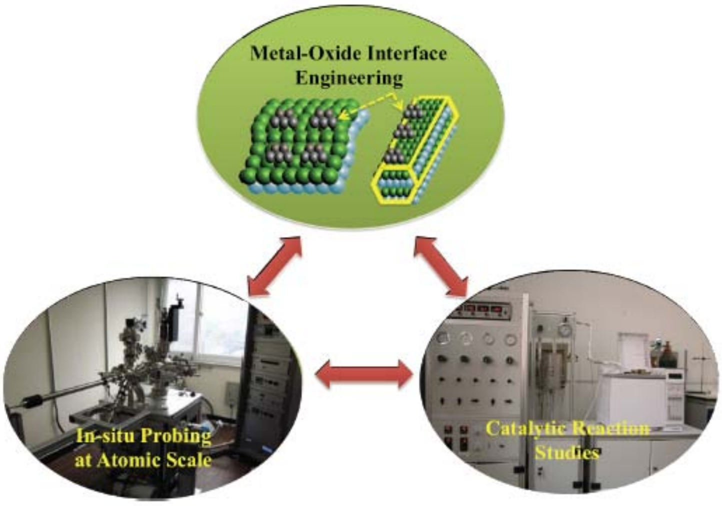

Figure: Summary scheme of the Research Program

2. Feasibility Analysis

2.1 Equipment and chemical reagents required for synthesis of the nano-catalysts: Basic equipment and chemical reagents provided by CRC (Catalytic Reaction Chemistry) Group at Dalian Institute of Chemical Physics (DICP) such as 1. Teflon lined Autoclaves, Magnetic Stirrers, Temperature controlled oil bath, glassware etc.

2.2 Equipment and Instruments required for Characterization of the nano-catalysts: The instruments required for basic analysis of nanocatalysts such as Catalyst Analyzer (Pulse Chemisorption measurement), BET Surface area measurement, instruments required for crystal structure, phase, composition, surface analysis such as High Resolution Scanning electron microscope (TEM) and Transmission electron microscope, X-Ray Diffraction, X-Ray photoelectron spectroscopy can be accessed inside DICP. Equipment required for Insitu analysis of nano-catalysts under reaction/gaseous conditions such as Environmental TEM can be accessed in DICP, while ambient pressure Scanning-tunneling microscope (STM) can be accessed in Professor Jeong Young Park's group at Korea Advanced Institute of Science and Technology (KAIST), South Korea.

博士后工作的研究计划

3. Expected Outcomes

• Our work is expected to generate novel and interesting results as currently, there is sparse reports existing on the subject of ultra-small nano-rods and nano-sheets of atomic dimensions with uniform size observed for ZnO, Ga2O3 and In2O3.

• It is expected that strong metal-support interaction (SMSI effect) will be observed clearly in our Metal-Oxide nanocatalysts due to ultra-small nano-scale dimensions of the nanocatalysts arising from unique electronic and geometric properties in contrast to bulk counterparts.

• It is expected that well-controlled Metal-Oxide based nanocatalysts will reveal clearly the contribution of perimeter interface area towards catalytic activity in Cu based nanocatalysts in particular and Metal NPs based nano-catalysts in general.

• It is also expected to open up a new field of investigation in nano-catalysis community investigating strong metal-support interactions in nano-catalysis in general and Cu based industrial catalysts such as Cu/ZnO/Al2O3 in particular. This will lead to bridging Materials gap between model studies and technological catalysts thereof.

4. Current progress

At present all experiments are designed and continually optimized. Literature survey in relationto synthesis of nano-rods and nano-sheets of ZnO has been completed and for Ga2O3 and In2O3 is being compiled. Additionally synthesis of ZnO nano-rod is in the process of optimization.

5. Challenges and Future Aspects

5.1 Challenges include:

• Preparation of ultra-small, uniform size nano-rods and nano-sheets of few atomic layer thickness of ZnO, Gallium oxide and Indium oxide.

• Fabrication of controlled interface in nanocatalysts.

• Probing interface perimeter active sites using environmental TEM and ambient pressure.

STM.

5.2 Future Aspects include:

• A novel route towards metal-oxide interface investigation and role in catalytic activity.

• It has the potential to be applied as a basic tool in catalysis to elucidate the metal-oxide interface effect in other similar catalytic systems.

• The insights gained can be applied to technological catalysts and therefore has direct significance to chemical technology industry thereby reducing the energy costs.

• This project in long run is a key way to bridge pressure and materials gap between model and real catalytic systems.

博士后工作的研究计划

6. Timetable of the Research Plan:

Time-line of the proposed project and brief research activity plan between 1st May 2016 ~ 31st April 2018 (2 years) is tabulated as following:

Duration of Project		Experiment Scheduled	Comments
Phase One Synthesis of ZnO, Ga_2O_3, In_2O_3 Nano-Rods and Nano-Sheets	**1st Quarter** From: 1st May 2016 To: 31st Oct 2016	(1) Synthesis of Rod Shaped ZnO, Incorporation of Cu NPs (2) Synthesis of Sheet Shaped ZnO, Incorporation of Cu NPs (3) Synthesis of Rod Shaped Ga_2O_3	(1) Chemical Synthesis route for Oxide, (2) Cu NPs of three different sizes (3) SEM/TEM as per requirement to optimize (4) XRD/XPS as per requirement to test crystal structure and oxidation states
	2nd Quarter From: 1st Nov 2016 To: 31st Apr 2017	(4) Synthesis of Sheet Shaped Ga_2O_3, Incorporation of Cu NPs (5) Synthesis of Rod Shaped In_2O_3, Incorporation of Cu NPs (6) Synthesis of Sheet Shaped In_2O_3, Incorporation of Cu NPs	
Phase Two In-situ/Ex-situ Characterization and Catalytic Reaction Test	**3rd Quarter** From: 1st May 2017 To: 31st Oct 2017	(7) HR- SEM to determine size and shape uniformity etc. (8) HR-TEM/ HAADF-STEM-EDS mapping images to determine lattice structure and perimeter interface contact lattice (9) Environmental TEM investigation of nanocatalysts under O_2/CO and CO, O_2 catalytic conditions	(5) Basic catalyst characterization techniques such as CO/H_2 pulse chemisorption as per need to evaluate metal NPs dispersion and surface area etc.
	4th Quarter From: 1st Nov 2017 To: 31st April 2018	(10) Ambient pressure STM of nanocatalysts under O_2/CO and CO, O_2 catalytic conditions (11) Analyzing and documenting data of key observations (12) Publishing key results and potential Patent registration of the nanocatalysts design method	(6) Ambient pressure STM to be carried out in Professor Jeong Young Park's group, South Korea, Collaboration agreed upon subject to sample provision

本人承诺

本人承诺：申请表所填内容均真实可靠。对因虚报、伪造等行为引起的后果及法律责任均由本人承担。

本人签字：　　　　　　　　　　　　年　　月　　日

博士后合作导师考核推荐表

对申请人学术水平、科研能力等方面的考核意见： Kamran Qadir 在韩国 Korea Advanced Institute of Science and Technology 攻读博士学位期间经过系统的训练，在催化剂制备、催化反应性能测试、催化剂结构分析和表征等方面积累了丰富的经验。并且能够熟练掌握多种催化表征常用仪器的操作，具备良好的独立科研能力和较高的学术水平。
对申请人提出的研究计划的评价（如可行性、先进性、创新之处、理论和实用意义）： Kamran Qadir 博士自加入大连化物所催化基础国家重点实验室从事博士后研究以来，在纳米催化剂的界面调控方面提出了一些创新性的研究思路和实验方案，有力推动了题目组相关研究工作的进展。Kamran Qadir 博士立意新颖、研究目标明确、实验方案设计细致，研 究方案切实可行、具有广阔的应用前景，具有较高的学术意义。
推荐意见（是否同意推荐申请优秀博士后奖励基金）： **我同意推荐他申请优秀博士后奖励基金**。 合作导师签字 年 月 日