# Dr. Yang Wang

Postdoctor,
Material Science and Technology Division
Oak Ridge National Laboratory
1 Bethel Valley Road
Oak Ridge, TN 37831, USA

Home Address:
9004C Creekside Lane,
Knoxville, Tennessee 37923

## Personal Information

Full Name: Yang Wang
Place of Birth: Xiangyang, China
Nationality: China
Phone(Mobile): +1-865-566-1026
Email: wangy1@ornl.gov / young.wang1983@gmail.com

## Education and Work Experience

| | | |
|---|---|---|
| **Postdoctor** | **Oak Ridge National Laboratory**<br>Supervisor: Dr. Paul Snijders, Prof. Hanno Weitering | ***Jul. 2014 – Present*** |
| **Technique Engineer** | **Oxford Instruments (Shanghai) Co, Ltd**<br>*Omicron NanoSciecne division* | ***Apr. 2013 – Jul. 2014*** |
| **Ph.D.** | ***Hefei National Lab for Physics Science at Microscale*, *University of Science and Technology of China***<br>*Atomic and Molecular Sciences*<br>Supervisor: Prof. Jianguo Hou, Prof. Bing Wang. | ***Sep. 2006 – Jun. 2013*** |
| **B.S.** | ***University of Science and Technology of China***<br>Condensed Matter Physics, | ***Sep. 2002 – Jun. 2006*** |

## Publications

1. **Yang Wang**, Huijuan Sun, Shijing Tan, Hao Feng, Zhengwang Cheng, Jin Zhao, Aidi Zhao, Bing Wang, Yi Luo, Jinlong Yang, J.G. Hou, ***Nature Communications*** (2013), 4:2214
2. **Yang Wang**, Zhengwang Cheng, Shijing Tan, Xiang Shao, Bing Wang , J.G. Hou, ***Surface Science*** (2013), 616,93
3. **Yang Wang,** Xiang Shao, Bing Wang, ***Acta Phys. -Chim. Sin***.(2013)**,** *29*, 1363
4. Shijing Tan, Hao Feng, Yongfei Ji, **Yang Wang**, Jin Zhao, Aidi Zhao, Bing Wang, Yi Luo, Jinlong Yang, J. G. Hou, ***Journal of the American Chemical Society*** (2012), 134, 9978
5. Zhi Li, Guanzhong Wang, Qianhui Yang, Zhibin Shao, **Yang Wang**, ***Nanoscale Research Letters*** ( 2012), 7:316

## Conference and Poster Presentations:

1. **Yang Wang,** Paul Snijders, Hanno Weitering, Preparing of atomicly flat $TiO_2$(001), APS March Meeting 2015, San Antonio, TX, USA

2. **Yang Wang,** Huijuan Sun, Hao Feng, Bing Wang, Jianguo Hou, Investigation of surface defects and adsorption behaviors of small molecules on anatanse $TiO_2$(001) single crystal films, CPS Fall Meeting 2012, Guangzhou, China

3. **Yang Wang**, Hao Feng. Bing Wang, Jianguo Hou, Preparing and characterization of Cr-N codoping antanse $TiO_2$ single crystal films, CPS Fall Meeting 2011, Hangzhou, China

## Reviewed Papers:

1. The influence of metal nanoparticles on electrical properties of carbon nanotubes, Applied Surface Science 2016
2. The study of the silicon dioxide anti-reflection film prepared by the sol-gel method, CMSE 2015
3. Influence of lateral growth on the surface pits of GaN heteroepitaxial film grown by MOCVD, CMSE 2015

4. Elements diffusion of the interface for Be/ 00Cr17Ni14Mo2 stainless steel by hot pressing, CMSE 2015
5. Influence of dopants ratio on structure and optical properties of N-Fe co-doped TiO2 films prepared via sol-gel dip-coating, CMSE 2015
6. Investigation on the water vapor oxidation of Super304H at 600℃, CMSE 2015
7. Synthesis and visible light photocatalytic activity of BiVO4/P25, CMSE 2015

## Researches and study

*As a Ph.D. Candidate from 2006 to 2013, my research project was preparing single crystal metal-oxide films by pulse laser deposition(PLD) and studied their chemical and physical properties via X-ray diffraction(XRD), scanning tunneling microscopy(STM), spin-polarized STM, ultraviolet photoelectron spectroscopy(UPS), X-ray photoelectron spectroscopy(XPS) and angle resolved photoelectron spectroscopy( ARPES). Undoped anatase $TiO_2$(001) and CrN-codoped anatase $TiO_2$(001) films have been prepared to study their photocatalytic activity. Doped manganites (LCMO and LPCMO) films have been prepared to study phase separation and percolation in strong correlation system.*

*Being a postdoctor since 2014, my interest is focused on heterostructures of transition metal oxide in rutile structre. Due to the strong correlations between 3d electrons of transition metal, rutile structures could undergo a phase transition from metal to insulator ($VO_2$) or ferromagnet to insulator ($MnO_2$). However, the mechanism driving the transition is still an open question. My project is prepare atomically flat rutile $TiO_2$ substrate and subsequently deposit $VO_2$, $CrO_2$ or $NbO_2$ films by MBE. The surface morphology, band structure, transport property will be investigated by STM, UPS and PPMS, respectively. These experiments will shed some light on elucidating the mechanism for phase transition.*

### 1: Study of reconstructions, defects and adsorption activities of molecules on atomic-flat anatase $TiO_2$(001)-1×4 thin films.

The chemical reactivity of different surfaces of titanium dioxide ($TiO_2$) has been the subject of extensive studies in recent decades. The anatase $TiO_2$(001) and its (1X4) reconstructed surfaces were theoretically considered to be the most reactive and have been heavily pursued by synthetic chemists. However, the lack of direct experimental verification or determination of the active sites on these surfaces has caused controversy and debate. Here we report a systematic study on an anatase $TiO_2$(001)-(1X4) surface by means of microscopic and spectroscopic techniques in combination with first-principles calculations. Two types of intrinsic point defects are identified, among which only the Ti3t defect site on the reduced surface demonstrates considerable chemical activity. The perfect surface itself can be fully oxidized, but shows no obvious activity. Our findings suggest that the reactivity of the anatase $TiO_2$(001) surface should depend on its reduction status, similar to that of rutile $TiO_2$ surfaces. (**Yang Wang**, Huijuan Sun, Shijing Tan, Hao Feng, Zhengwang Cheng, Jin Zhao, Aidi Zhao, Bing Wang, Yi Luo, Jinlong Yang, J.G. Hou, ***Nature Communications*** (2013), 4:2214)

### 2: Characterization of Cr–N codoped anatase $TiO_2$(001) thin films epitaxially grown on $SrTiO_3$(001) substrate.

We investigate the growth of Cr–N codoped anatase $TiO_2$(001) thin films, prepared with a pulsed-laser-deposition (PLD)method using amixed $Cr_2O_3$ and TiN ceramic target (6 at.% Cr), and characterized using scanning tunneling microscopy (STM), X-ray and ultraviolet photoemission spectroscopy (XPS/UPS), and ultraviolet–visible (UV–Vis) absorption spectroscopy. We find that the doping concentration of N in the films can be finely tuned by the $O_2$ pressure and the growth temperature. By optimizing the growth conditions, we obtain the anatase $TiO_2$(001) films with relatively smooth (1 × 4) reconstructed surface at equally codoped contents of 6 at.% Cr and 6 at.% N. The roughness of the surface is about 0.9 nm in root mean square, and the typical size of the (1 × 4) terraces is about 20 nm. The XPS results indicate that Cr and N should be both substitutionally doped in the film. From the UPS spectrum for the codoped film, the valence band maximum is significantly lifted by about 1.3 eV, indicating a narrowing band gap of 1.9 eV. The optical absorption spectrum shows that the codoped film noticeably absorbs the light at less than

710 nm. Derived from the optical absorption spectrum, an estimated band gap value of 1.78 eV is obtained, which is consistent with the UPS result. (**Yang Wang**, Zhengwang Cheng, Shijing Tan, Xiang Shao, Bing Wang , J.G. Hou, ***Surface Science*** (2013), 616,93)

### 3: Preparation, characterization and photocatalytic activity of Cr-Doped rutile TiO2(110) Single crystal thin films.

The growth of Cr-doped rutile TiO2(110) homoepitaxial single crystal thin films using the pulsed laser deposition (PLD) method was investigated. Surface morphology and electronic structure were characterized using scanning tunneling microscopy/spectroscopy (STM/STS), and X-ray and ultraviolet photoemission spectroscopies (XPS/UPS). Optical absorption spectra were measured using ultravioletvisible (UV-Vis) absorption spectroscopy. STM images revealed that the atomically flat $TiO_2$(110)-(1 × 1) surface was maintained at a Cr doping concentration of 6% (atomic ratio), indicating that the Cr dopant had negligible effect on surface morphology. The Cr-doped rutile $TiO_2$(110) film showed higher tunneling conductance than an undoped rutile single crystal. XPS and UPS spectra indicated that Cr atoms bound to lattice O, were present in +3 oxidation state and introduced an impurity state 0.4 eV above the valence band maximum. The UV-Vis absorption spectrum of the Cr-doped film showed an absorbance extending to ~650 nm in the visible range, which was consistent with UPS measurements. Using the Cr-doped $TiO_2$ films, the dissociation of methanol molecules was only observed under irradiation with UV light (wavelength shorter than 430 nm). The dissociation reaction was not observed under irradiation with visible light (wavelength longer than 430 nm). Our results suggest that doping with Cr element alone may not be sufficient to promote the visible light photoactivity of rutile $TiO_2$(110) surfaces. ( **Yang Wang,** Xiang Shao, Bing Wang, ***Acta Phys. -Chim. Sin***.(2013)**,** *29*, 1363)

### 4: Observation of photocatalytic dissociation of water on terminal Ti sites of $TiO_2$(110)-1 × 1 surface.

The water splitting reaction based on the promising $TiO_2$ photocatalyst is one of the fundamental processes that bears significant implication in hydrogen energy technology and has been extensively studied. However, a long-standing puzzling question in understanding the reaction sequence of the water splitting is whether the initial reaction step is a photocatalytic process and how it happens. Here, using the low temperature scanning tunneling microscopy (STM) performed at 80 K, we observed the dissociation of individually adsorbed water molecules at the 5-fold coordinated Ti (Ti5c) sites of the reduced $TiO_2$ (110)-1 × 1 surface under the irradiation of UV lights with the wavelength shorter than 400 nm, or to say its energy larger than the band gap of 3.1 eV for the rutile $TiO_2$. This finding thus clearly suggests the involvement of a photocatalytic dissociation process that produces two kinds of hydroxyl species. One is always present at the adjacent bridging oxygen sites, that is, $OH_{br}$, and the other either occurs as $OH_t$ at Ti5c sites away from the original ones or even desorbs from the surface. In comparison, the tip-induced dissociation of the water can only produce OHt or oxygen adatoms exactly at the original Ti5c sites, without the trace of $OH_{br}$. Such a difference clearly indicates that the photocatalytic dissociation of the water undergoes a process that differs significantly from the attachment of electrons injected by the tip. Our results imply that the initial step of the water dissociation under the UV light irradiation may not be reduced by the electrons, but most likely oxidized by the holes generated by the photons. **(**Shijing Tan, Hao Feng, Yongfei Ji, **Yang Wang**, Jin Zhao, Aidi Zhao, Bing Wang, Yi Luo, Jinlong Yang, J. G. Hou, ***Journal of the American Chemical Society*** (2012), 134, 9978)

### 5: Synthesis and electrical property of metal/ZnO coaxial nanocables.

Ag/ZnO and Cu/ZnO coaxial nanocables were fabricated using $AgNO_3$ or copper foil as source materials by the vapor-liquid-solid process. The coaxial nanocables consist of a crystalline metallic Ag or Cu core and a semiconductor ZnO shell. The evolution of the Ag/ZnO products having different morphologies was investigated by stopping the heating at different temperatures. The diameters of the Ag/ZnO nanocables and the Ag cores could be modulated by changing Ag ratio in the source. The electrical characteristics of the Ag/ZnO contact and the influence of annealing reveal a Schottky diode behavior for a single Ag/ZnO nanocable device. The nanocables with uniform shape and controlled size are expected to provide a new choice in various applications of biological detection, nanothermometer, and photocatalysis. **(**Zhi Li, Guanzhong Wang, Qianhui Yang, Zhibin Shao, **Yang Wang**, ***Nanoscale Research***

***Letters*** ( 2012), 7:316)