Final Report for Research Grant 16-399

Research Grant Reference 16-399

Project Title: ***"A novel nanostructured SiC electrode for solar fuel development"***

2019-12-06

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Summary:

In order to solve the energy and environmental problems such as the exhaustion of traditional fossil fuels, and ever more evident environmental impact of air pollutants and CO_2, both academic and industrial research efforts in finding alternate renewable energy sources are dramatically increased over the last decades. *The photoelectrochemical (PEC) water splitting* into *solar fuels* such as H_2 and methanol using sunlight has attracted much attention because of its potential to use the abundance of solar energy and water on Earth. This project focuses on development of SiC materials as the photoelectrode to convert solar energy into chemical fuels.

In this project, we have built a solar water splitting measurement setup and a PhD student has participated in the project and has received his PhD degree on 2019-09-12. Moreover, a postdoc researcher has been recruited and has been working in this project since 2017-09-01. We have successfully fabricated high-quality C-face and Si-face 3C-SiC, graphene on 3C-SiC, nanostructured 3C-SiC and demonstrated their promising properties on solar-to-fuel conversion (see the PhD dissertation and publication list below). In particular, we have demonstrated that the bottleneck of photoelectrochemical water oxidation can be overcome via atomic manipulation of proton transfer on the polar surfaces of SiC photoanodes. Furthermore, we improved the solar water splitting efficiency by introducing electrocatalytic and p-type NiO nanoclusters on an n-type cubic silicon carbide (3C-SiC) photoanode. Under AM1.5G 100 mW/cm^2 illumination, the nanostructured NiO-coated 3C-SiC photoanode exhibits a significantly increased photocurrent and photovoltage together with decreased on-set potentials. More detailed results have been published in Yuchen Shi's PhD thesis and our papers (see below).

PhD Dissertation and Published papers with support of this project:

PhD Dissertation:

Yuchen Shi, " Growth of 3C-SiC and Graphene for Solar Water-Splitting Application", ***the PhD Dissertation, 12 September 2019.***

Publications:

[1]. Weimin Wang, Yuchen Shi, Alexei A Zakharov, Mikael Syväjärvi, Rositsa Yakimova, Roger IG Uhrberg, **Jianwu Sun*,** *"Flat-band electronic structure and interlayer spacing influence in rhombohedral four-layer graphene",* ***Nano letters, 18, 5862-5866, (2018).***

[2]. Yuchen Shi, Valdas Jokubavicius, Pontus Höjer, Ivan G Ivanov, G Reza Yazdi, Rositsa Yakimova, Mikael Syväjärvi and **Jianwu Sun*,** "A comparative study of high-quality C-face and Si-face 3C-SiC(1 1 1) grown on off-oriented 4H-SiC substrates", ***J. Phys. D: Appl. Phys. 52 345103, (2019)***

[3]. Yuchen Shi, Alexei A Zakharov, Ivan G Ivanov, G Reza Yazdi, Valdas Jokubavicius, Mikael Syväjärvi, Rositsa Yakimova, **Jianwu Sun*,** *"Elimination of step bunching in the growth of large-area monolayer and multilayer graphene on off-axis 3CSiC (111)",* ***Carbon, 140, 533-542, (2018).***

[4]. Jingxin Jian, Yuchen Shi, Mikael Syvajarvi, Rositsa Yakimova, and **Jianwu Sun*,** "*Cubic SiC Photoanode Coupling with Ni:FeOOH Oxygen-Evolution Cocatalyst for Sustainable Photoelectrochemical Water Oxidation*" ***SOLAR RRL 2019, 1900364***.

[5]. Jingxin Jian, Yuchen Shi, Sebastian Ekeroth, Julien Keraudy, Mikael Syväjärvi, Rositsa Yakimova, Ulf Helmers-son and **Jianwu Sun*, "***A nanostructured NiO/cubic SiC p–n heterojunction photoanode for enhanced solar water splitting*", ***Journal of Materials Chemistry A, 7, 4721–4728, (2019).***

[6]. Hao Li, Huan Shang, Yuchen Shi, Rositsa Yakimova, Mikael Syväjärvi, Lizhi Zhang, and **Jianwu Sun*,** "*Atomically manipulated proton transfer energizes water oxidation on silicon carbide photoanodes*", ***Journal of Materials Chemistry A, 6, 24358-24366, (2019).***

[7]. Xiang Ao, Jianjun Jiang, Yunjun Ruan, Zhishan Li, Yi Zhang, **Jianwu Sun,** Chundong Wang, "*Honeycomb-inspired design of ultrafine SnO2@C nanospheres embedded in carbon film as anode materials for high performance lithium- and sodium-ion battery*", ***Journal of Power Sources, 359, 340-348, (2017).***

[8]. Jianwu Sun gave a popular presentation entitled " Direct Conversion of Solar Energy into Fuels" on Feb. 8th, 2017 in the EWEEK Conference (http://eweek.nu/index.php/program).

> EWEEK is an annual conference and meeting place for regional and national participants in the energy and environmental sector. E-Week is gathering experts, officials, policy makers and researchers to discuss solutions for a sustainable future. E-Week also aims to give the region's entrepreneurs knowledge of energy and climate, which they can use to increase their profitability.

Jianwu Sun organized conferences:

- **Organizer** of the 2nd workshop of NACSiC (New applications of cubic silicon carbide workshop), December 14-15, 2016, Linköping University, Sweden.

- **Co-organizer** of Symposium E3: "Materials for Energy harvesting" in EUROMAT 2017 (European Congress and Exhibition on Advanced Materials and Processes), Thessaloniki, Greece, from 17 – 22 September, 2017.