

4<sup>th</sup> International Conference on **Electrochemistry**

June 11-12, 2018 | Rome, Italy

**Interfacially engineering topological semimetal MoP into a superior electrocatalyst for hydrogen evolution**Guowei Li<sup>1</sup>, Gudrun Auffermann<sup>1</sup>, Claudia Felser<sup>1</sup> and Xinliang Feng<sup>2</sup><sup>1</sup>Max Planck Institute for Chemical Physics of Solids, Germany<sup>2</sup>Technische Universität Dresden, Germany

Materials in topological states are endowed with many exotic properties such as extremely large magnetoresistance, high conductivity, and intrinsic Hall effects. However, the effect of such appealing properties on electrocatalysis still remains elusive. Recently, the observation of exceedingly high conductivity and Weyl nodes in MoP provide us with a modeling catalyst for revealing the correlation between topological states and electrocatalytic activity and designing high-performance electrocatalyst for hydrogen evolution reaction (HER). MoP encapsulated in Mo, P co-doped carbon layer (MoP@C) was thus synthesized and exhibits outstanding electrocatalytic HER performance with an extremely low overpotential of only 49 mV at a current density of 10 mA/cm<sup>2</sup> and a decreased Tafel slope of 54 mV/dec. in alkaline medium. Such superior HER activity of the MoP@C exceeds those of the state-of-art non-noble metal-based HER electrocatalysts and even comparable to that of the Pt/C catalyst. As a topological semimetal, MoP manifests a very high conductivity (8.2 μΩ at 300 K) and mobility (up to 10 cm<sup>2</sup>/VS at 300 K) due to the topologically protected triple point fermions and complex Fermi surface. Meanwhile, the rich P-C and Mo-C bonds in the interfaces between the carbon layer and MoP modulates the band structure of MoP@C and eventually facilitates the fast electron transfer, accumulation, and subsequent de-localization, which are responsible for the excellent HER activity.

**Recent Publications**

1. G Li, G R Blake and T T M Palstra (2017) Vacancies in functional materials for clean energy storage and harvesting: the perfect imperfection. *Chem. Soc. Rev.* 46:1693-1706.
2. G Li, B Zhang, T Baluyan, J Rao, J Wu, A A Novakova, P Rudolf, G R Blake, R de Groot and T T M Palstra (2016) Metal insulator transition induced by spin reorientation in Fe<sub>7</sub>Se<sub>8</sub> grain boundaries. *Inorg. Chem.* 55:12912-12922.
3. G Li, R Su, J Rao, J Wu, P Rudolf, G R Blake, R de Groot, F Besenbacher and T T M Palstra (2016) Band gap narrowing of SnS<sub>2</sub> superstructures with improved hydrogen production. *J. Mater. Chem. A* 4:209-216.
4. G Li, B Zhang, J Rao, D Gonzalez, G R Blake, R Groot and T T M Palstra (2015) Effect of vacancies on magnetism, electrical transport, and thermoelectric performance of marcasite FeSe<sub>2-δ</sub> (δ=0.05). *Chem. Mater.* 27(24):8220-8229.
5. G Li, B Zhang, F Yu, A A Novakova, M S Krivenkov, T Y Kiseleva, L Chang, J Rao, A O Polyakov, G R Blake, R de Groot and T T M Palstra (2014) High purity Fe<sub>3</sub>S<sub>4</sub> greigite microcrystals for magnetic and electrochemical performance. *Chem. Mater.* 26(20):5821-5829.

**Biography**

Guowei Li received his Master's degree in Materials Science from Jiangsu University in 2011 with Prof. Changsheng Li. He then moved to the University of Groningen, the Netherlands, and was awarded the PhD degree under the supervision of Dr. Graeme R Blake and Prof. Thomas T M Palstra in 2016. Since then, he joined the Max Planck Institute for Chemical Physics of Solids, Dresden as a Postdoctoral Fellow in the group of Prof. Claudia Felser. His research interests focus on the magnetic and electrical transport properties of chalcogenides and topological materials, from synthesis to applications in clean energy harvesting and conversion.

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