Rapid Communication

Symbiotic CeH$_{2.73}$/CeO$_2$ catalyst: A novel hydrogen pump

Huai-Jun Lin$^{a,d}$, Jia-Jun Tang$^{a,c}$, Qian Yu$^{b,e,*}$, Hui Wang$^{a}$, Liu-Zhang Ouyang$^{a}$, Yu-Jun Zhao$^{c}$, Jiang-Wen Liu$^{a}$, Wei-Hua Wang$^{d,**}$, Min Zhu$^{a,***}$

$^a$School of Materials Science and Engineering, South China University of Technology, Key Laboratory of Advanced Energy Storage Materials of Guangdong Province, Guangzhou 510640, PR China
$^b$National Center for Electron Microscopy, Lawrence Berkeley National Laboratory, Berkeley, CA 94720, United States
$^c$Department of Physics, South China University of Technology, Guangzhou 510640, PR China
$^d$Institute of Physics, Chinese Academy of Sciences, Beijing 100080, PR China
$^e$Center of Electron Microscopy and State Key Laboratory of Silicon Materials, Department of Materials Science and Engineering, Zhejiang University, Hangzhou 310027, PR China

Received 14 April 2014; received in revised form 16 June 2014; accepted 24 June 2014
Available online 15 July 2014

Abstract
Using additives/catalysts to destabilize hydrides of high hydrogen storage density, e.g. MgH$_2$ with 7.6 wt%-H and desorption temperature as high as 300–400 °C, is one of the most important strategies to overcome the hurdle of applying hydrogen storage materials in technologies related to hydrogen energy. Despite tremendous efforts, to develop additives/catalysts with high catalytic activity and easy doping remains a great challenge. Here, we report a simple method to induce a novel symbiotic CeH$_{2.73}$/CeO$_2$ catalyst in Mg-based hydrides, which is capable of massive fabrication. More importantly, we reveal a spontaneous hydrogen release effect at the CeH$_{2.73}$/CeO$_2$ interface, which leads to dramatic increase of catalysis than either sole CeH$_{2.73}$ or CeO$_2$ catalyst. Maximum hydrogen desorption temperature reduction of MgH$_2$ could reach down to ~210 °C as molar ratio of CeH$_{2.73}$ to CeO$_2$ was 1:1. The dynamic boundary evolution during hydrogen desorption was observed in the symbiotic CeH$_{2.73}$/CeO$_2$ at atomic resolution using in situ High-Resolution Transmission Electron Microscope (HRTEM). Combining the ab-initio calculations, which show significant reduction of the formation energy of V$_{H}$ (hydrogen vacancy) in the CeH$_{2.73}$/CeO$_2$ boundary region in comparison to those in the bulk.

Key words: Hydrogen storage; MgH$_2$; Symbiotic CeH$_{2.73}$/CeO$_2$; Catalysis; In situ HRTEM; Theoretical calculations

http://dx.doi.org/10.1016/j.nanoen.2014.06.026
2211-2855/© 2014 Elsevier Ltd. All rights reserved.
MgH₂ and CeH₂.73, we demonstrate that the outstanding catalytic activity can be attributed to the spontaneous hydrogen release effect at the CeH₂.73/CeO₂ interface. © 2014 Elsevier Ltd. All rights reserved.

Introduction

Hydrogen, as an ideal fuel for future clean and renewable energy system, will hardly be practically applied if it could not be safely stored in appropriate way [1-3]. Solid-state hydrogen storage materials, e.g. MgH₂ with hydrogen storage density of ~7.6 wt%, are widely considered as promising carriers for hydrogen storage. However, temperature as high as 300-400 °C is generally required for desorption of MgH₂ due to the stable thermodynamics and sluggish kinetics [4]. Therefore, exploring advanced catalysts plays important role for the development of high capacity hydrogen storage materials. Catalysts doping by methods of ball milling and chemical process, very often together with nanoscaling, is a vital way to compensate the kinetic drawbacks [5]. Transition metals [6], chlorides [7], hydrides [8] and oxides [9,10] etc. have been found to present catalytic activity for de/hydrogenation of Mg-based materials, which might be driven from the “hydrogen spillover” effect [11,12], electron transfer of the high-valence cations [13,14], formation of anion-containing species [7] or MgH₂ catalysts interface reaction [15] etc. Direct evidence is highly demanded to clarify and understand the intrinsic catalysis, which is unfortunately not available so far.

Another critical issue raised is in the practical doping process of catalysts in hydrogen storage materials. Generally speaking, sophisticated chemical synthesis process and ball milling are commonly adopted. Although the former one can lead to excellent de/hydrogenation kinetics, it is usually not suitable for massive production plus the requirement of extra treatment for polluted chemical agents [16,17], while the later one is also associated with the difficulty of the control of size and distribution of the catalysts. In addition, contamination harmful to materials is easily induced by atmosphere and milling debris in the long-time process. Therefore, to develop easy and effective doping strategy of catalyst, capable of massive fabrication in the hydrogen storage materials with well-controlled structure and distribution is crucial for optimal catalyzing effect and presumably has strong impact on the practical application of catalysts doped hydrogen storage materials.

In this work, we propose a simple strategy to generate a novel symbiotic CeH₂.73/CeO₂ catalyst in Mg-based hydrides with controlled size by simple conventional hydriding and heat treatment process exempting long-time ball milling and sophisticated chemical process. In situ HRTEM characterizations during dehydrogenation were performed together with ab-initio calculations to reveal the catalysis. A spontaneous hydrogen release effect (corresponding to negative formation energy of V_H) in the CeH₂.73/CeO₂ interface is responsible for the improvement of the dehydrogenation of MgH₂.

Experimental details

Materials synthesis

Preparation details of the amorphous Mg–Ce–Ni ribbons are described elsewhere [18,19]. The amorphous ribbons with composition of M₈₈₀Ce₁₀Ni₁₀ were crushed via ball milling (200 rpm) for only 2 h into powder, and then screened through 200 mesh sieves. After that, the powder was thermally activated under hydrogen gas of 10 MPa at 300 °C for 3 h and then treated by 15 times dehydrogenated and rehydrogenated at 300 °C for 0.5 h under 0.02 and 3 MPa hydrogen gas, respectively. Then, the 15th cycled sample was placed in an Ar-atmosphere glove box for around 1 week (passivation treatment). Finally, about 0.30 g sample was sealed in a tube (2 ml) full of air at room temperature for 1, 5, 8 and 20 h to obtain the MgH₂-Mg₈Ni₅H₁₄-CeH₂.73/CeO₂ nanocomposites with different molar ratios of CeO₂ to CeH₂.73.

Characterizations

Common phase analysis and in situ high-temperature X-ray diffraction (XRD) analysis were conducted on a Philips XPert MPD X-ray diffractometer with Cu Kα radiation. Conventional transmission electron microscopy (TEM) and high resolution transmission electron microscopy (HRTEM) observations were carried out on a JEOL JEM-2100 microscope with 200 kV voltage. The in situ TEM measurements were performed in a TECNAI microscopes with the Gatan heating holders. The samples were heated up to about 300 °C. The electron beam heating also contributes to the increase of temperature. Scherzer resolution of the TECNAI is 0.19 nm, and information limit is 0.12 nm. Differential scanning calorimetry (DSC) tests were carried out on a Netzsch STA-409 analyzer; the separation (peak deconvolution) was done using the PeakFit 4.12 software with a Gaussian response function. TPD-MS analysis was performed on a Hiden Qic-20 mass spectrometer. Hydrogenation/dehydrogenation kinetics and cycles tests were performed on a Sieverts-type automatic gas reaction controller (Pct Pro2000). The sample weight for hydrogen storage property test was around 100 mg.

Theoretical calculations

Our theoretical calculations were performed using Vienna ab-initio Simulation Package [20-22]. We applied the spin-polarized density-functional theory (DFT) in the DFT+U approach (U is a Hubbard-like term describing the onsite Coulomb interactions) with the PBE (Perdew-Burke-Ernzerhof) functional [23] and projector-augmented wave (PAW) potentials [24]. For cerium and oxygen atoms, the (5s, 5p, 6s, 4f,
CeO₂ is formed from CeH₂.₇₃ and the molar ratio of CeO₂ get a multiphase composite of MgH₂, Mg₂NiH₄ and CeH₂.₇₃ with energy convergence to be in precision of ~0.001 eV per cell and the plane-wave cutoff energy was set to be 400 eV. The internal optimization was converged with the force on each atom to be less than 0.01 eV/Å. The CeH₆(111)/CeO₂(111) (x=2, 2.25, 2.5, 2.75 and 3) interfaces were modeled using a supercell containing two phases where each phase with three layers (shown in Figure 4c). The calculated CeO₂, CeH₂, CeH₂.₇₅ and CeO₃ bulk equilibrium lattice constant were 5.492 Å, 5.415 Å, 5.507 Å and 5.429 Å, respectively. Considering slight differences between these lattice constants, we built a (2x2) coherent interface model, with 24 cerium atoms, 24 oxygen atoms and 12x hydrogen atoms (x=2, 2.25, 2.5, 2.75 and 3) and lattice constants of 5.51 Å. Test calculations indicated that convergence problem occurred when the interface model was with vacuum. Therefore, the model was built having two identical interfaces without vacuum. All atoms in models were allowed to relax with the interface unit cell kept fixed during geometry optimization.

Results and discussion

Materials synthesis

The process of inducing symbiotic CeH₂.₇₃/CeO₂ catalyst in the MgH₂ matrix is shown in Figure 1. The first step is to hydrogenate the amorphous Mg-Ce-Ni alloy (Figure 1a) to get a multiphase composite of MgH₂, Mg₃NiH₄ and CeH₂.₇₃ (Figure 1b). The second step is to oxidize the hydrogenated sample to generate CeO₂ from CeH₂.₇₃ (Figure 1c). The transition process of the microstructure in the above treatment process is revealed by the X-ray diffraction (XRD) analyses, which are shown in the insets of Figure 1. The CeO₂ is formed from CeH₂.₇₃ and the molar ratio of CeO₂ to CeH₂.₇₃ could be determined by oxidation process. The ratio is ~1:1 in the situation of ~8 h oxidation at 25 °C. It is significant that Gibbs free energy ΔG of the reaction CeH₂.₇₃+O₂→CeO₂+H₂ at 25 °C is −1423 kJ while that of the reaction MgH₂+O₂→MgO+H₂ at 25 °C is −1066 kJ [27]. Thus, only CeO₂ could be induced with exclusion of MgO formation under suitable control of oxidation process.

In order to reveal the structural relationship between CeH₂.₇₃ and CeO₂, TEM and HRTEM observations are performed as shown in Figure 2. Figure 2a shows the HRTEM image of the typical symbiotic structure of the CeO₂/CeH₂.₇₃ nanoparticles, and they can also form core-shell structure as shown in Figure 2b and c. Since the lattice parameters of CeH₂.₇₃ (space group: Fm-3m, a=0.5530 nm, PDF 89-3694) and CeO₂ (space group: Fm-3m, a=0.5412 nm, PDF 81-0792) are extremely close, we performed HRTEM images, FFT patterns and also EDS analysis to confirm that CeO₂ was epitaxially formed from CeH₂.₇₃ in a cubic to cubic orientation relationship. More microstructural characterizations for the MgH₂-Mg₃NiH₄-CeH₂.₇₃/CeO₂ composite are given in Figures S1 and S2.

Hydrogen desorption

The MgH₂-Mg₃NiH₄-CeH₂.₇₃/CeO₂ composite displays remarkable reduction of hydrogen desorption temperature compared with that of the conventional MgH₂. It is important to note that this is highly related to the ratio of CeH₂.₇₃ to CeO₂ (Figure S3). With the increase of that ratio, the hydrogen desorption temperature decreases at first and then increases after reaching the trough at the molar ratio of 1:1. We suppose that the catalytic activity of the symbiotic CeH₂.₇₃/CeO₂ might have close relationship with their interface density, which reaches the maximum when molar ratio of CeH₂.₇₃ to CeO₂ is 1:1, however, the mechanism is not well understood. The lowest dehydrogenation onset temperature, as determined by DSC measurement, is only ~210 °C at the presence of the symbiotic CeH₂.₇₃/CeO₂, which is ~210 °C lower than that of conventional MgH₂ (Figure 3a). In order to reveal the detailed evolution of phases of the MgH₂-Mg₃NiH₄-CeH₂.₇₃/CeO₂ nanocomposite with molar ratio of CeH₂.₇₃ to CeO₂ of 1:1 during hydrogen desorption, in situ XRD measurements are carried out as shown in Figure 3b. Surprisingly, desorption of MgH₂ starts at almost the same temperature as Mg₃NiH₄. It indicates that the formation of symbiotic CeH₂.₇₃/CeO₂ nanoparticles.
diffraction patterns during dehydrogenation. It can be clearly seen that the diffraction intensity of Mg increasingly enhances as desorption time prolongs, indicating the decomposition of MgH₂. The dynamic evolution of the interface structure of the symbiotic CeH₂.73/CeO₂ during dehydrogenation is studied via in situ HRTEM studies. Figure 4a presents the microstructural evolution of the typical symbiotic CeH₂.73/CeO₂ nanocrystals during dehydrogenation. Interestingly, the boundary region suffers severe distortions and the distorted area fluctuates wave-like during hydrogen desorption, suggesting that the interface region of the symbiotic nanocrystals undergoes structural evolution at atomic scale, which presumably plays a prominent role for hydrogen releasing in dehydrogenation.

Detailed animation could refer to Supplementary Video S1. To further understand the evolution of interface and the origin of the intrinsic catalysis, theoretical calculations are performed to reveal the catalysis induced from the symbiotic CeH₂.73/CeO₂. Since the higher catalytic effect of the symbiotic CeH₂.73/CeO₂ on dehydrogenation of MgH₂ compared to that of Mg₂NiH₄, our calculations focus on the MgH₂-CeH₂.73/CeO₂, and the results are discussed in the following section.

Supplementary material related to this article can be found online at http://dx.doi.org/10.1016/j.nanoen.2014.06.026.

Theoretical calculations

We begin with the analysis of the formation energy of V_H in MgH₂, which could be significantly affected by the valence state variations (Figure S7a). The V_H is with the lowest formation energy of 1.35 eV among three vacancy types considered when the Fermi energy is around 3 eV. The formations of V_H and V_H⁺ are more energetically favored than V_H when the Fermi energy ranges from 0 to 2.76 eV and from 3.08 to 4.5 eV respectively, indicating that the V_H valence state variations influence the V_H formation. The large areas of V_H⁺ and V_H in Figure S7b indicate the energetic preference of high-concentration V_H formation. It has been reported that the V_H formation energy in CeO₂ could be reduced when there are empty orbitals lower than 4f of cerium [31]. For the MgH₂/CeO₂ interface, the Fermi
level of MgH$_2$ could be raised as oxygen vacancies often provide electrons to the Fermi sea of the system, leading to a much lower formation energy of V$_{\text{H}}$. Thus we suppose that hydrogen release would firstly happen in the MgH$_2$/CeO$_2$ interface and then hydrogen would migrate towards and across CeO$_2$ due to the role of CeO$_2$ as efficient vector for hydrogen diffusion [32].

We use the Climbing Image Nudged Elastic Band (CI-NEB [33,34]) to analyze the hydrogen migration barriers in three types of CeO$_2$, including pure CeO$_2$ (Type 1), CeO$_2$ with V$_{\text{O}}$ (Type 2) and CeO$_2$ with V$_{\text{H}}$ site partially occupied by hydrogen (Type 3), and the results are shown in Table S1. Figure 4b shows that the hydrogen migration in Type 1 is nearly barrierless (0.09 eV and 0.17 eV) since the hydrogen migration between ‘hydroxyl’ structures are quite easy [35]. We notice that the hydrogen migration could be remarkably influenced by V$_{\text{O}}$. Specifically, hydrogen migration near V$_{\text{O}}$ might be attracted and tends to take up the V$_{\text{O}}$ site with an energy barrier of 0.83 eV. The trap of hydrogen at V$_{\text{O}}$ sites is locally stable since the energy barrier for hydrogen departure from the occupied V$_{\text{O}}$ site is 1.09 eV. However, it does not affect the nearly barrierless migration of hydrogen in CeO$_2$ since the number of V$_{\text{O}}$ is rather limited. In addition, we consider hydrogen migration barriers in two configurations of CeO$_2$ with V$_{\text{O}}$ site partially occupied by hydrogen (c.f. Figure 4b). The formation energies of two structures are $-0.36 \, \text{eV}$ and $0.69 \, \text{eV}$. The large difference of formation energy of 1.05 eV indicates that the hydrogen ‘dimer’ structure is not energetically favored. In our NEB calculations, the hydrogen connected to H$_{\text{OC}}$ (hydrogen at oxygen site) could depart spontaneously, which is manifested by the negative energy barrier, suggesting that the H$_{\text{OC}}$ could not be able to trap hydrogen to form H-dimer. Furthermore, due to the limited concentration of H$_{\text{OC}}$, the dominating mechanism of hydrogen migrations in Type 3 is the same as in Type 1 where hydrogen migrates easily between ‘hydroxyl’ structures. In short, CeO$_2$ could serve as a good transporter for hydrogen migration.

Next, the formation energies of V$_{\text{H}}$ in the CeH$_x$/CeO$_2$ ($x=2, 2.25, 2.5, 2.75$ and $3$) interface region have been conducted to investigate the interfacial effects in comparison with the bulk cases. Although there are several possible configurations of the CeH$_{2.75}$/CeO$_2$ interface, we found that the CeH$_{2.75}$/CeO$_2$ interface would take an O-Ce-H configuration (Figure 4c) due to its lowest interfacial energy ($-0.32 \, \text{eV/Å}^2$) rather than the others, i.e. H-Ce-Ce-O (not stable) and Ce-O-H-Ce ($-0.25 \, \text{eV/Å}^2$). The O-Ce-H configuration is adopted in CeH$_x$/CeO$_2$ interfaces for comparison. Single and double V$_{\text{H}}$ and V$_{\text{O}}$ at different sites in the interface region are considered. Table S2 lists the formation energies of different types of V$_{\text{H}}$ and V$_{\text{O}}$ at the CeH$_x$/CeO$_2$ ($x=2, 2.25, 2.5, 2.75$ and $3$) interfaces and in the bulk CeH$_x$ ($x=2.25, 2.5, 2.75$ and $3$). The formation energy of V$_{\text{O}}$ at the CeH$_{2.75}$/CeO$_2$ interface is lowered to 2.06 eV compared to 2.91 eV in CeO$_2$ bulk, indicating that there might be the release of small amount of O$_2$ at the interface region (Figure S8). When $x$ is less than 2.75, the formation of V$_{\text{O}}$ becomes more difficult, which is reflected by the 2.89 eV of CeH$_{2.25}$/CeO$_2$ and 3.19 eV of CeH$_{2.5}$/CeO$_2$. Furthermore, the energetic advantage of V$_{\text{O}}^{\text{ex}}$ in three interfaces is in agreement with the previous papers [36,37], which proposed that the formation of V$_{\text{O}}$ in second layer facilitates the atom

![Image](https://example.com/image.png)
relaxations and electron localization that lead to system stability. The formation of $V_O$ provides excess electrons which might facilitate the hydrogen desorption in MgH$_2$. The calculated CeH$_3$ bulk is found to exhibit a Ce–H$_t$ (tetrahedral H) bond of 2.34 Å and a Ce–H$_o$ (octahedral H) bond of 2.71 Å. The difference of the bond strength, which has also been observed in the lanthanum hydride [38], illuminates the possibility of easier Ho desorption due to the weaker Ce–Ho bonding. Our calculations of formation energies of $V_H$ imply that the CeH$_{2.75}$/CeO$_2$ interface could be able to serve as an efficient “hydrogen pump”. On one hand, the $V_{Ho}$ at the CeH$_{2.75}$/CeO$_2$ interface is quite energetically unfavored. Specifically, single and double $V_{Ho}$ are found to form spontaneously, reflected by negative formation energies even at the H-rich condition. The double vacancies $V_{Ho}^{1st} + V_{Ho}^{1st}$ and $V_{Ho}^{1st} + V_{Ho}^{2nd}$, which includes the concern of $V_{Ho}$, are also with low formation energies of 0.22 and 0.24 eV, respectively. On the other hand, the formation energies of single vacancy $V_{Ho}^{1st}$ and $V_{Ho}^{2nd}$ and double vacancies $V_{Ho}^{1st} + V_{Ho}^{2nd}$ are in quite low level, namely 0.16, 0.17 and 0.06 eV, respectively, which might lead to an easy release of hydrogen as temperature increases. Moreover, the instability of CeH$_3$ indicates that it is difficult for hydrogen accumulation at the CeH$_x$/CeO$_2$ when $x$ reaches 2.75. We attribute this to the instability of Ho of CeH$_{2.75}$ (the light gray atoms in Figure 4c). In contrast, the high stability of CeH$_2$, which arises from the stable bonding between cerium and Ht, implies that the hydrogen desorption at interface requires more energy as the hydrogen concentration is lowered. In the CeH$_2$/CeO$_2$,
CeH$_{2.75}$/CeO$_2$ and CeH$_{2.73}$/CeO$_2$ interfaces, the formation energies of $V_{H}$ are all higher than those of the CeH$_{2.75}$/CeO$_2$ interface. Compared to the octahedral $V_{H}$ formation energies in Ce$_3$ bulk, the $V_{H}$ formation energies at the CeH$_{2.75}$/CeO$_2$ interface are significantly decreased. In short, the interfacial effect of CeH$_{2.75}$/CeO$_2$ is capable of serving as an efficient “hydrogen pump” where excess hydrogen would be released very easily.

Conclusions

In summary, the hybrid of CeH$_{2.73}$ and CeO$_2$ with low catalytic effect exhibits surprisingly high catalytic activity for dehydrogenation of MgH$_2$. We show that the $V_{H}$ formation in MgH$_2$ can be stimulated by electron transfer from CeO$_2$, and the CeO$_2$ is capable of transporting hydrogen to the CeO$_2$/CeH$_{2.73}$ interface where the release of hydrogen is quite easy. The spontaneous hydrogen release effect in the interface region of the symbiotic CeO$_2$/CeH$_{2.73}$ nanoparticles accounts for its role of efficient “hydrogen pump”. The symbiotic CeH$_{2.73}$/CeO$_2$ catalyst is suitable for large-scale productions due to the easy fabrication technology. Our findings might open a novel approach to explore the advanced catalysts for alloy-based hydrogen storage materials.

Acknowledgments

This work was financially supported by the Ministry of Science and Technology of China (No. 2010CB631302), the National Natural Science Foundation of China (Nos. U1201241, 51071068 and 51271078) and KLGEHI (KBL11003) and the Fundamental Research Funds for the Central Universities.

Appendix A. Supporting information

Supplementary data associated with this article can be found in the online version at http://dx.doi.org/10.1016/j.nanoen.2014.06.026.

References

[27] Database from HSC6.0 Software.
Qian Yu received her Ph.D. at University of California Berkeley in 2012, she is currently a post-doc at University of California Berkeley and Lawrence Berkeley National Laboratory. Dr. Yu has been interested in in situ transmission electron microscope characterization on materials properties.

Hui Wang received his B.S. degree in Metal Materials, Tianjin University in 1997, and Ph.D. degree in Material Science and Engineering, South China University of Technology (SCUT) in 2003. He is currently an associate professor in SCUT. His research focuses on hydrogen storage materials, microstructure analysis by X-ray diffraction with Rietveld method, non-equilibrium state synthesis of metastable materials etc.

Liu-Zhang Ouyang received his B.S. degree in Materials Science, Yanshan University in 1994, and Ph.D. degree in Material Science and Engineering, South China University of Technology (SCUT) in 2001. He is currently a professor in SCUT. His research focuses on hydrogen storage materials, hydrogen generation and lithium ion battery materials. He has published more than 100 papers in international journals.

Jiang-Wen Liu received his B.S. degree in Materials Science and Engineering, Shanghai Jiaotong University in 1987, and Ph.D. degree in Materials Science and Engineering, South China University of Technology (SCUT) in 1998. He is currently a professor in SCUT. His research focuses on nanomaterials and their nanostructure-property relationship through characterizing nanomaterials using electron microscopy, hydrogen storage materials, and lithium ion battery materials.

Wei-Hua Wang is a professor of Institute of Physics, Chinese Academy of Sciences at Beijing, China. His research focuses on the formation, structure, physical properties and glass transition in metallic glasses. He earned his Ph.D. degree in condensed matter physics at Chinese Academy of Sciences in 1993, and was Humboldt fellow in 1995-1997. He has published more than 100 papers in international journals.

Yu-Jun Zhao received his B.S. degree (1994) and Ph.D. degree (1999) in physics at Zhejiang University. Since then, he has been a post-doc at Northwestern University and National Renewable Energy Laboratory, and a researcher at Nanostellar Inc. at Silicon Valley. Dr. Zhao joined South China University of Technology (SCUT) in 2006 as a professor of physics, and is currently the group leader of Computational Physics for Condensed Matters at SCUT. Dr. Zhao has been interested in crystal defect theory and surface science, with research topics including magnetic semiconductors, surface catalysis, photovoltaic materials, and hydrogen storage materials.

Min Zhu is a professor in South China University of Technology (SCUT). He received his Ph.D. from Dalian University of Technology in 1988. He worked in the Technical University of Berlin as a Humboldt Research Fellow in 1993-1995. He was appointed as a “Cheung Kong Professor” in 2002. Prof. Zhu is working in the fields of hydrogen storage materials, lithium ion battery materials, shape memory alloys and mechanical alloying, and published more than 200 papers.