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에너지융합기술 혁신인재 양성사업단

Innovative Education & Research Center for Energy Convergence Science and Technology

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KIT Energy 소식

신소재공학부 학부생, 재료 분야 최고 수준 국제학술지 연이어 게재

-공동 제1저자(4학년 최선연·석사과정 김선우 학생) 논문
-'새로운 이차원 반도체 물질 합성 및 트랜지스터 소자제작 기술'개발

신소재공학부 4학년 최선연·석사과정 김선우 학생(지도교수 김현호)이 공동 제1저자로 참여한 논문이 재료 분야의 국제 저명 학술지에 게재됐다.

논문 제목은 'Understanding Solvent-Induced Delamination and Intense Water Adsorption in Janus Transition Metal Dichalcogenides for Enhanced Device Performance(야누스 전이금속 칼코게나이드 물질기반 소자의 성능 향상을 위한 용매에 의한 박리와 높은 물 흡착의 이해)'로, SCI급 국제학술지인 'Advanced Functional Materials(상위 5%, IF 19.924)'온라인판에 11월 12일 자로 게재됐다. 오프라인으로는 오는 12월에서 1월 중 게재될 예정이다.

최선연 학생은 앞서 8월에도 '산화그래핀 기반 물리적 복제방지 보안기술'논문을 동일 학술지 'Advanced Functional Materials'에 제1저자로 게재한 바 있다. 이번 논문은 이를 이은 두 번째 논문으로 학부생이 제1저자로 주도한 연구결과가 국제 저명 SCI급 학술지에 연이어 게재된 것은 주목할 성과다.

김선우 학생과 최선연 학생은 Janus(야누스) 구조를 가진 전이금속 칼코겐화합물(TMDC)인 Janus MoSSe에 대한 연구를 진행했다. TMDC는 이차원 소재 가운데 전이금속 원소 하나를 기준으로 위아래에 칼코겐족 원소 두 개가 위치하여 X-M-X 구조(예: Se-Mo-Se)의 대칭적인 구조를 하고 있지만, Janus TMDC의 경우 서로 다른 칼코겐족 원소 두 개가 비대칭적인 X-M-Y 구조(예: S-Mo-Se)로 되어 있다. 이에 Janus MoSSe는 기존 TMDC 물질의 장점 외에도 압전 효과와 우수한 촉매성 등의 높은 잠재력을 가지고 있어 최근 큰 주목을 받고 있다.

그러나 높은 잠재력을 가진 Janus MoSSe는 쌍극자 모멘트가 존재하여 극성 용매에 의한 박리와 수분 흡착에는 취약한 특징 때문에 반도체 소자제작 공정에 활용하기에는 어려움이 있었다. 이러한 문제를 해결하기 위해 본 연구에서는 Janus MoSSe 하단 및 상단에 절연 재료(h-BN)를 사용하여 반 데르 발스 이종 구조를 기반으로 하는 전계 효과 트랜지스터를 제작하여 향상된 전자 이동도와 우수한 안정성을 나타냈다.

김선우, 최선연 학생은 "처음 이 연구를 시작할 때 Janus MoSSe를 기반으로 한 소자제작에 어려움을 가졌지만 Janus MoSSe 물질이 가진 독특한 특성을 이해하고 관련 문제를 해결하며 많은 것을 배우게 됐다."며, "앞으로도 다양한 연구를 통해 반도체소자 분야의 연구를 이끌어나가는 세계적인 인재가 되고 싶다."고 밝혔다.

지도교수인 김현호 교수는 "Janus TMDC 소재는 이론적으로는 다양한 가능성을 가지고 있지만 이에 대한 실험적인 구현은 아직 초기 단계"라며, "학생들이 Janus TMDC 소재 기반 소자 응용에 대해 보다 깊이 이해하고 활용할 수 있도록 함께 연구 활동을 이어가겠다."고 밝혔다.

이번 연구는 신소재공학부 저차원 나노소재 및 반도체소자 연구실 주도를 통해 수행됐으며, 교육부 4단계 BK21사업, 과학기술정보통신부 우수신진연구, 미래기술연구실 등의 지원으로 수행됐다.

금오공과대학교 KIT People(2023.11.21.) https://www.kumoh.ac.kr/ko/sub01_05_02.do?mode=view&articleNo=469602

◈ 관련 기사 ◈

경북매일신문	금오공대 신소재공학부 학부생, 국제학술지 연이어 게재	http://www.kbmaeil.com/news/articleView.html?idxno=975598
베리타스알파	금오공대 신소재공학부 학부생 재료 분야 최고 수준 국제학술지 연이어 게재	http://www.veritas-a.com/news/articleView.html?idxno=482397
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매일신문	금오공대 신소재공학부 학부생, 최고 수준 국제학술지 연이어 게재	https://www.imaeil.com/page/view/2023112117075744980
교수신문	국립금오공대 신소재공학부 학부생, 재료 분야 최고 수준 국제학술지 연이어 게재	http://www.kyosu.net/news/articleView.html?idxno=112505
경상매일신문	국립금오공대 신소재공학부 학부생, 재료 분야 최고 수준 국제학술지 연이어 게재	http://www.ksmnews.co.kr/news/view.php?idx=455103
전자신문	금오공대 학부생, 이차원 반도체 물질 합성 및 트랜지스터 소자제작 기술 개발 …SCI급 학술지에 게재	https://www.etnews.com/20231121000137
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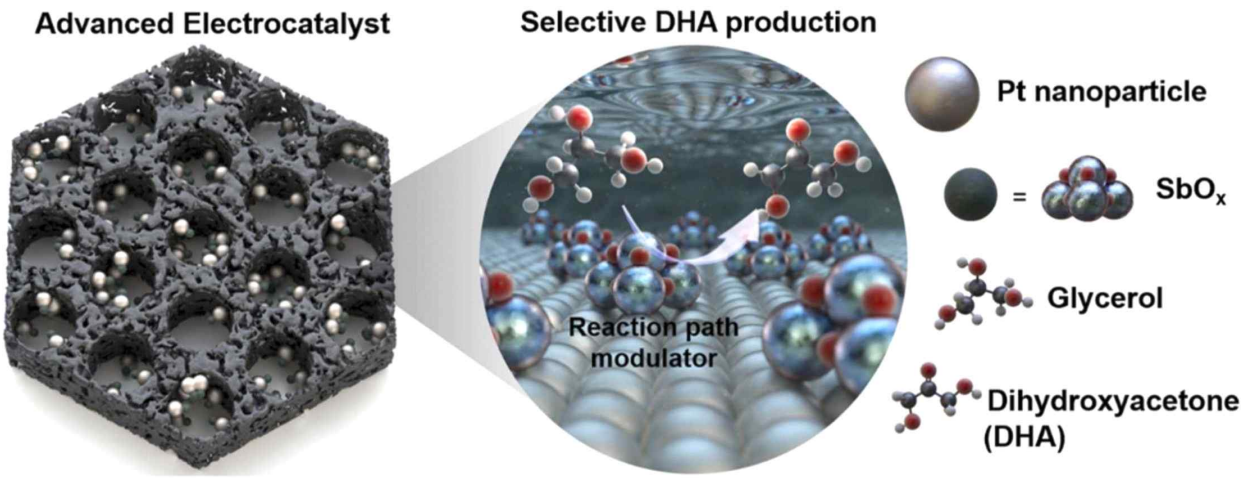
수소에너지

Applied Catalysis B: Environmental
Volume 339, December 15, 2023, p123104 (Impact Factor : 22.1)

Amorphous antimony oxide as reaction pathway modulator toward electrocatalytic glycerol oxidation for selective dihydroxyacetone production

Dongkyu Kim, Won-Gwang Lim, Youngmin Kim, Lee Seul Oh, Seongseop Kim, Jong Hyeok Park, Changshin Jo, Hyung Ju Kim, Joonhee Kang*, Seonggyu Lee*, Eunho Lim*



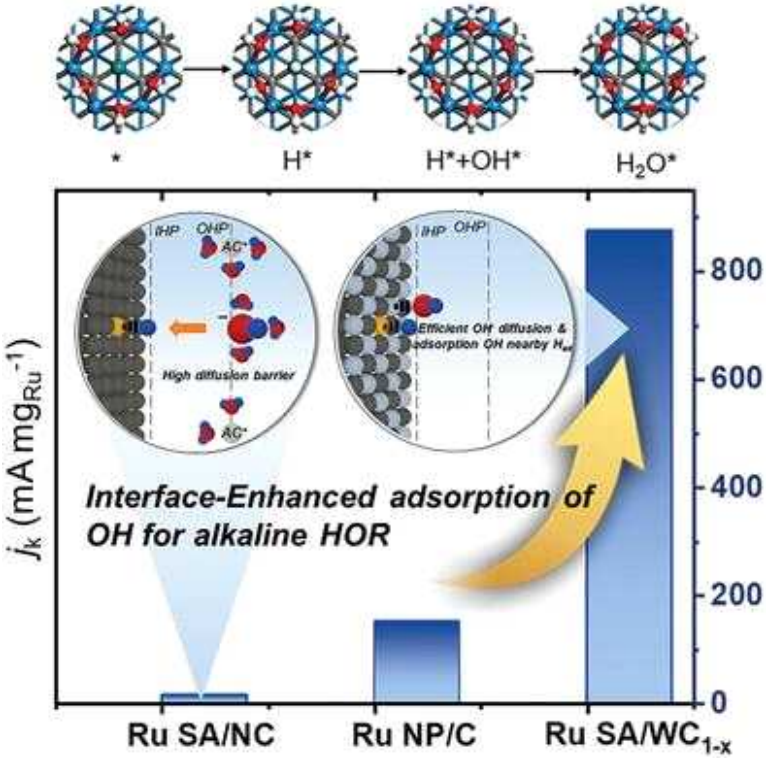
Achievement of an efficient and stable electrocatalytic glycerol oxidation reaction (EGOR) is limited by a lack of strategies for designing advanced electrocatalysts that satisfy the desired product selectivity, high electrocatalytic activity, and stability. Here, we report that the reaction pathway of EGOR can be modulated by the incorporation of amorphous antimony oxide (SbOx) on the surface of a Pt nanoparticle electrocatalyst (SbOx-Pt), which creates highly selective glycerol oxidation to dihydroxyacetone (DHA), one of the most valuable products of EGOR. The selective control of adsorption behaviors of glycerol oxidation products allows for SbOx to act as a reaction pathway modulator. Moreover, SbOx deposition on a Pt surface also enhances the stability, electrocatalytic activity, and glycerol conversion of the Pt electrocatalyst, and thus promotes the EGOR. As a result, the SbOx-Pt electrocatalyst achieves a high DHA selectivity of 81.1%, which is about 11 times higher than that of commercial Pt/C electrocatalysts.

수소에너지

Advanced Materials
November 11, 2023 (온라인 게재) (Impact Factor : 29.4)

Boosting Alkaline Hydrogen Oxidation Activity of Ru Single-Atom Through Promoting Hydroxyl Adsorption on Ru/WC1−x Interfaces

Jinkyu Park, Honghui Kim, Seongbeen Kim, Seung Yeop Yi, Hakyung Min, Daeeun Choi, Seonggyu Lee, Jihan Kim*, Jinwoo Lee*



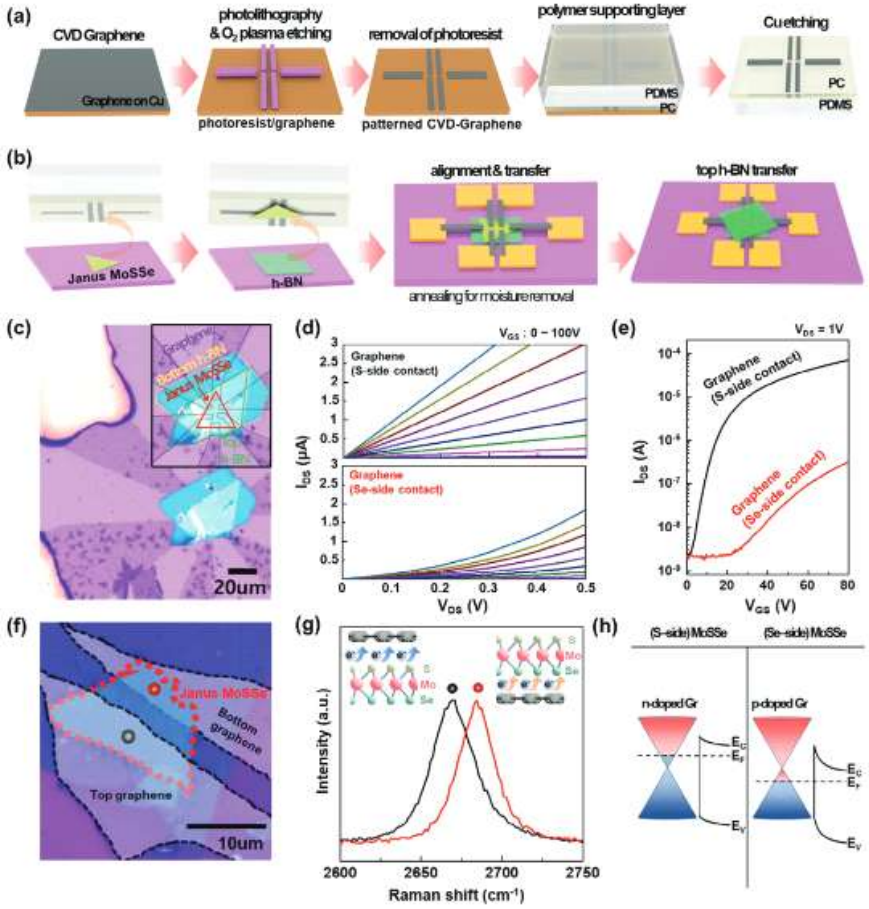
The sluggish kinetics of the hydrogen oxidation reaction (HOR) in alkaline conditions continue to pose a significant challenge for the practical implementation of anion-exchange membrane fuel cells. Developing single-atom catalysts can accelerate the pace of new HOR catalyst discovery for highly cost-effective and active HOR performance. However, single-atom catalysts (SACs) for the alkaline HOR have rarely been reported, and fundamental studies on the rational design of SACs are still required. Herein, the design of Ru SAC supported on the tungsten carbide (Ru SA/WC1−x) via in situ high-temperature annealing strategy is reported. The resulting Ru SA/WC1−x catalyst exhibits remarkably enhanced HOR performance in alkaline media, a level of activity that can not be achieved with carbon-supported Ru SAC. Electrochemical results and density functional theory demonstrate that promoting the hydroxyl adsorption on Ru SA/WC1−x interfaces, which is derived from the low potential of zero charge of WC1-x support, has a significant effect on enhancing the HOR performance of SACs. This enhancement leads to 5.8 and 60.1 times higher Ru mass activity of Ru SA/WC1−x than Ru nanoparticles on carbon and Ru single-atom on N-doped carbon, respectively. This work provides new insights into the design of highly active SACs for alkaline HOR.

에너지변환

Advanced Functional Materials
Issue 2308709, November 2023 (온라인게재) (Impact Factor : 19.0)

Understanding Solvent-Induced Delamination and Intense Water Adsorption in Janus Transition Metal Dichalcogenides for Enhanced Device Performance

Sun Woo Kim, Seon Yeon Choi, Si Heon Lim, Eun Bee Ko, Seunghyun Kim, Yun Chang Park, Sunghun Lee, Hyun Ho Kim*



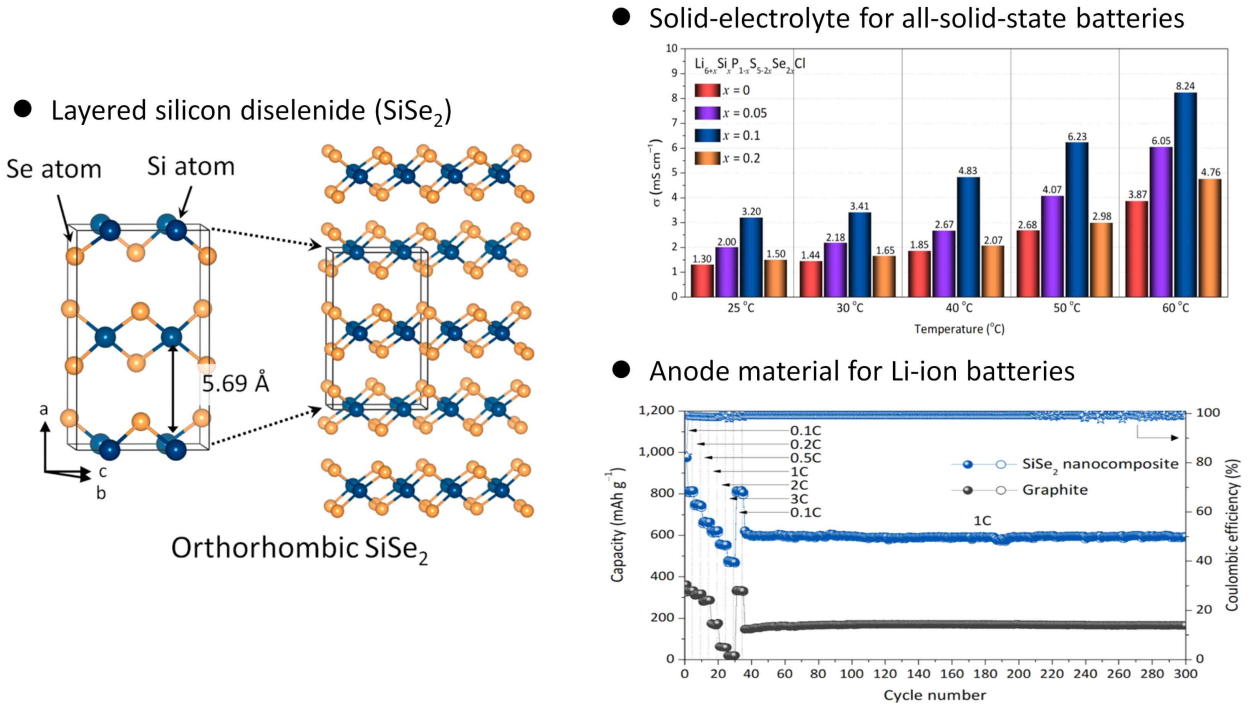
Recently, there has been considerable interest in 2D Janus transition metaldichalcogenides owing to their unique structure that exhibits broken mirrorsymmetry along the out-of-plane direction, which offers fascinating propertiesthat are applicable in various fields. This study investigates the issue ofprocess instability in Janus MoSSe, which is mainly caused by its nonzero netdipole moments. It systematically investigates whether the built-in dipolemoments in Janus MoSSe make it susceptible to delamination by most polarsolvents and increase its vulnerability to intense moisture adsorption, whichleads to the deterioration of its semiconducting properties. To address theseissues, as an example of device applications, field-effect transistors (FETs)based on a van der Waals heterostructure are devised, where the bottom h-BN(top h-BN) insulating material is employed to prevent delamination(adsorption of moisture). The fabricated FETs exhibit improved electronmobility and excellent stability under ambient conditions.

에너지저장

ACS Applied Materials & Interfaces
Online Published, December 2023, Accepted (Impact Factor : 9.5)

$SiSe_2$ for Superior Sulfide Solid Electrolytes and Li-Ion Batteries

Ki-Hun Nam, Vinoth Ganesan, Do-Hyeon Kim, Sangmin Jeong,
Ki-Joon Jeon*, Cheol-Min Park*



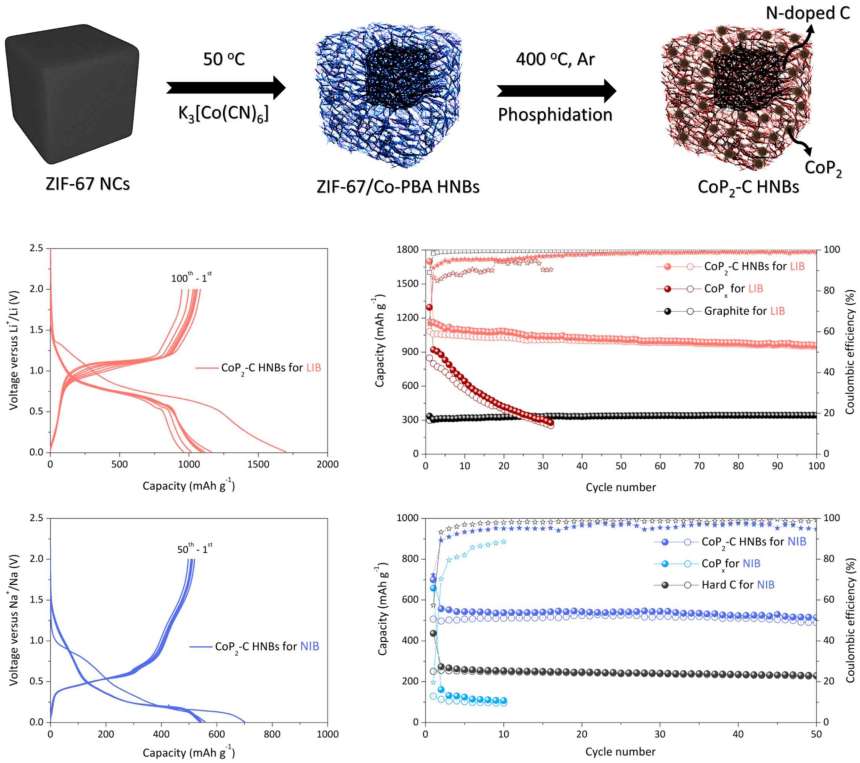
Among the various existing layered compounds, silicon diselenide ($SiSe_2$) possesses diverse chemical and physical properties, owing to its large interlayer spacing and interesting atomic arrangements. Despite the unique properties of layered $SiSe_2$, it has not yet been used in energy applications. Herein, we introduce the synthesis of layered $SiSe_2$ through a facile solid-state synthetic route and demonstrate its versatility as a sulfide solid electrolyte (SE) additive for all-solid-state batteries (ASSBs) and as an anode material for Li-ion batteries (LIBs). Li-argyrodites with various compositions substituted with $SiSe_2$ are synthesized and evaluated as sulfide SEs for ASSBs. $SiSe_2$-substituted Li-argyrodites exhibit high ionic conductivities, low activation energies, and high air stabilities. In addition, when using a sulfide SE, the ASSB full cell exhibits a high discharge/charge capacity of 202/169 mAh g^{-1} with a high initial Coulombic efficiency (ICE) of 83.7% and stable capacity retention at 1C after 100 cycles. Furthermore, the Li-storage properties of $SiSe_2$ as an anode material for LIBs are evaluated, and its Li-pathway mechanism is explored by using various cutting-edge *ex situ* analytical tools. Moreover, the $SiSe_2$ nanocomposite anode exhibits a high Li-insertion/extraction capacity of 950/775 mAh g^{-1}, a high ICE of 81.6%, a fast rate capability, and stable capacity retention after 300 cycles. Accordingly, layered $SiSe_2$ and its versatile applications as a sulfide SE additive for ASSBs and an anode material for LIBs are promising candidates in energy storage applications as well as myriad other applications.

에너지저장

Journal of Energy Storage
Online Published, December 2023, 110197 (Impact Factor : 9.4)

Robust CoP_2-C hollow nanoboxes: Superior anodes for Li- and Na-ion batteries

Vinoth Ganesan, Do-Hyeon Kim, Cheol-Min Park*



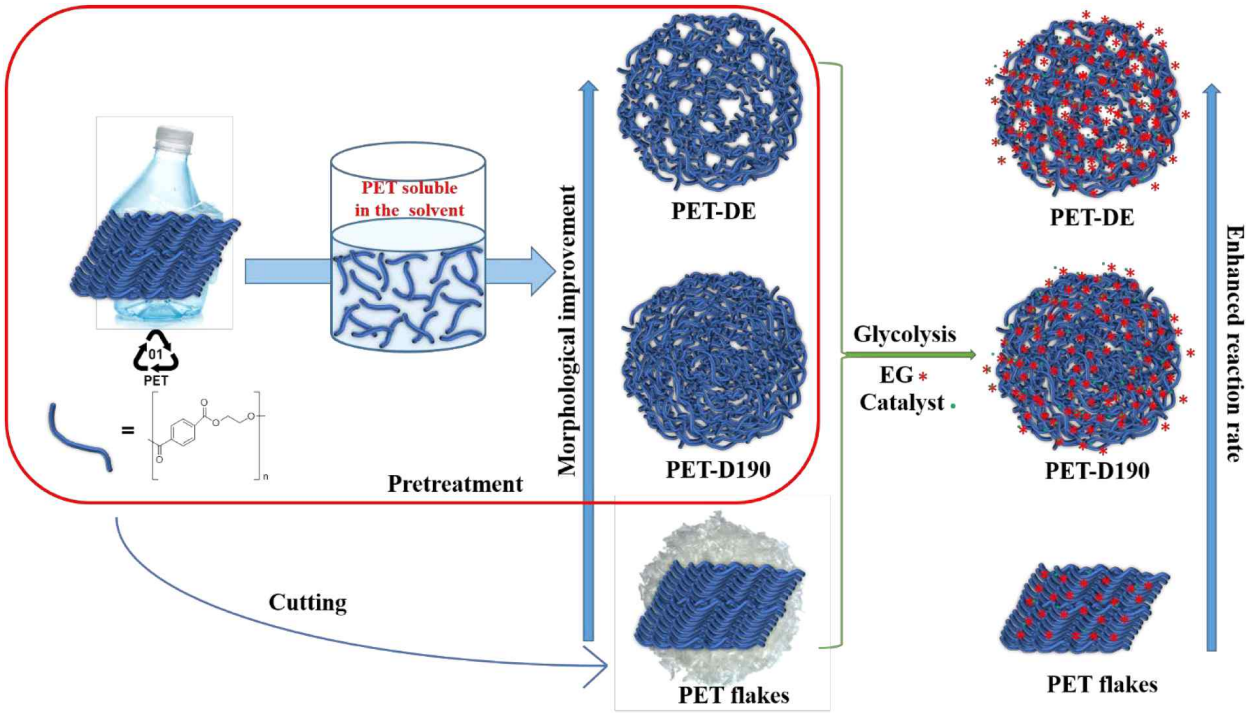
Metal phosphides are attractive candidates for use as anodes in high-performance Li/Na-ion batteries (LIBs/ NIBs) owing to their high theoretical capacities and low operating potentials. In this study, CoP_2-C hollow nanoboxes (HNBs), that is, CoP_2 nanocrystallites (~5–10 nm) embedded in N-doped carbon HNBs, were produced using a simple two-step method and utilized as LIB/NIB anodes. Various cutting-edge *ex situ* techniques were used to analyze the phase transition mechanism of the CoP_2-C HNBs during the Li/Na reaction. The CoP_2-C HNBs anode exhibited high initial reversible capacities (LIB: 1082 mAh g^{-1}, NIB: 507 mAh g^{-1}), high-rate capabilities (LIB: 926 mAh g^{-1} at 3C, NIB: 370 mAh g^{-1} at 2C), and excellent cycling performance at a high 1C rate (LIB: ~91 % capacity retention over 100 cycles, NIB: ~100 % capacity retention over 100 cycles), respectively. The excellent anode performance of LIBs/NIBs was attributed to the uniformly embedded CoP_2 nanocrystallites in the robust N-doped carbon HNBs and the electrochemically driven recombination reaction of CoP_2. Therefore, we believe that CoP_2-C HNBs are promising high-capacity anodes for LIBs/NIBs, and that this unique HNBs architecture is highly suitable for various energy storage and conversion systems.

에너지저장

Polymer Degradation and Stability
220, 2024, 12, 110649 (Impact Factor : 5.9)

Morphology control of waste polyesters for enhanced glycolysis reactivity and minimization of side reactions

Dieu Minh Ngo, Myeonggeun Jang, Hohyeon Noh, Hyun Min Jung*



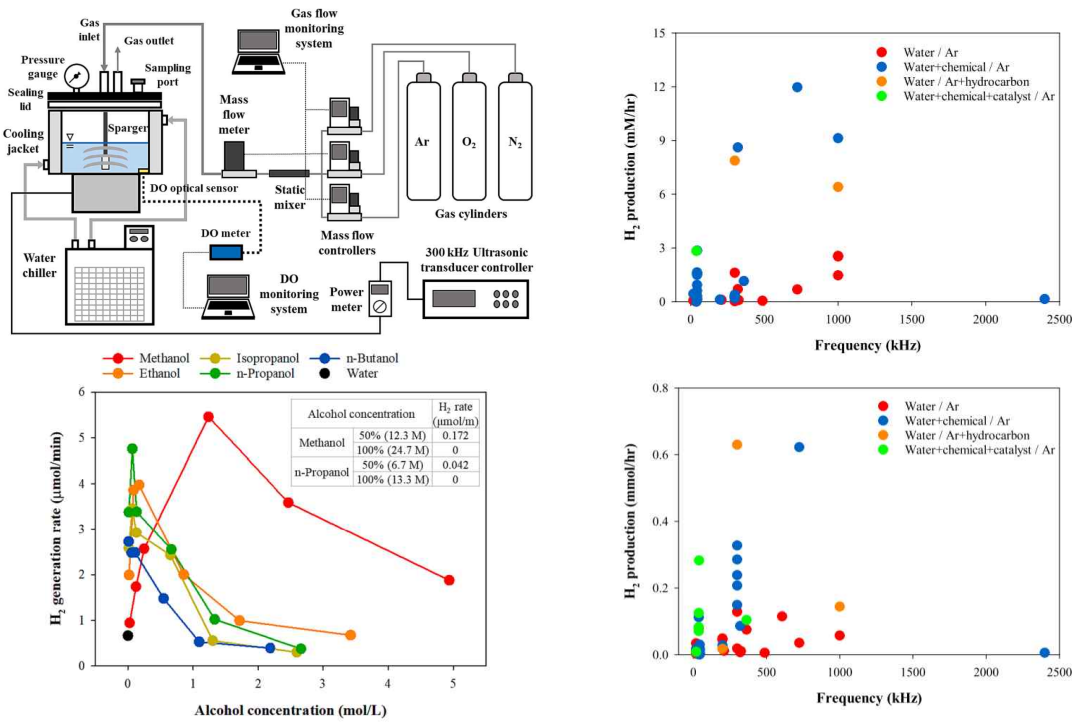
Effective pretreatment routes using dimethyl sulfoxide (DMSO) as solvent were accomplished to enhance the polyethylene terephthalate (PET) glycolysis rate. Highly ordered structure PET flakes were dissolved in DMSO at high temperatures, followed by solid-liquid separation using two different methods to generate micro-sized powders. Under identical glycolysis conditions, the reaction time of pretreated PET powders was gradually reduced by approximately five times that of PET flakes. During the glycolysis of PET with ethylene glycol (EG), diethylene glycol-containing terephthalate compounds (DCTC) are formed as undesired byproducts at high temperatures. These byproducts significantly affect the overall quality of BHET. Consequently, pretreated PET degradation under mild conditions was employed as a preventive measure against EG dehydration, leading to the production of DCTC. PET powders with controlled morphology exhibit outstanding performance and achieve a 100 % PET conversion at 180 ◦C to DCTC-free bis(2-hydroxyethyl) terephthalate (BHET). The purity of the obtained BHET was characterized using proton-NMR spectroscopy, Fourier transform infrared spectroscopy, and differential scanning calorimetry. The utilization of this technology presents a potential solution for overcoming the technical and economic challenges associated with current PET upcycling methodologies.

환경에너지

Ultrasonics Sonochemistry
Volume 101, December 2023, 106660 (Impact Factor : 8.4)

Effects of alcohols and dissolved gases on sonochemical generation of hydrogen in a 300 kHz sonoreactor

Jongbok Choi, Seokho Yoon, Younggyu Son*



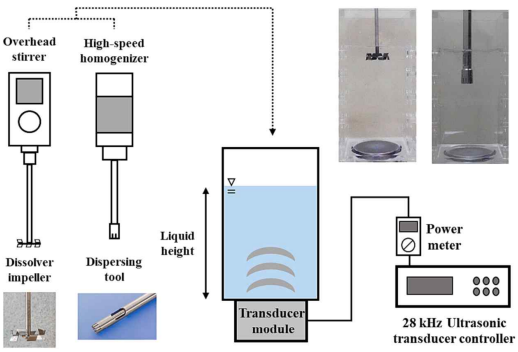
The sonochemical generation of hydrogen (H_2) was investigated using various water/alcohol solutions under argon (Ar) 100 % in a 300 kHz sonoreactor. Five types of alcohols-methanol, ethanol, isopropanol, n-propanol, and n-butanol-were used at various concentrations (0 - 100 % v/v). The H_2 generation rate in water was 0.31 μ mol/min in the absence of alcohols. The H_2 generation rate increased, peaked, and then decreased as the alcohol concentration increased. The concentrations used for the peak H_2 generation were 5 %, 1 %, 0.5 %, 0.5 %, and 0.1 % for methanol, ethanol, isopropanol, n-propanol, and n-butanol, respectively. The highest generation rate (5.46 μmol/min) was obtained for methanol 5 % among all conditions in this study, and no H_2 was detected for 100 % alcohol concentrations. The reason for the enhancement of the sonochemical H_2 generation by the addition of alcohols might be due to strong scavenging effect of alcohols for sonochemically generated oxidizing radicals and vigorous reactions of alcohol molecules and their derivatives with H radicals. No significant correlations were found between the H_2 generation rates and physicochemical properties of the alcohols in any of the data in this study. As alcohol concentration increased, the calorimetric power decreased. This indicates that the calorimetric power does not represent the degree of sonochemical reactions in the water/alcohol mixtures. The effect of oxygen (O_2) content in the dissolved gases on the generation of H_2O_2 (representing sonochemical oxidation activity) and H_2 (representing sonochemical reduction activity) was investigated using Ar/O_2 mixtures for water, methanol 5 % and n-propanol 0.5 %. In water, the highest H_2O_2 generation was obtained for Ar/O_2 (50:50), which is similar to previous research results. However, the H_2O_2 generation increased as the O_2 content increased. In addition, H2 generation decreased as the O_2 content increased under all liquid conditions (water, methanol, and n-propanol).

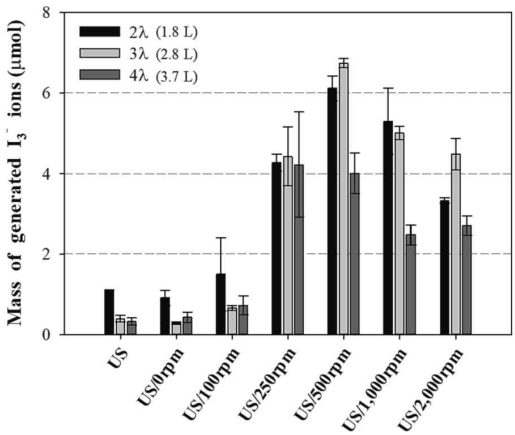
환경에너지

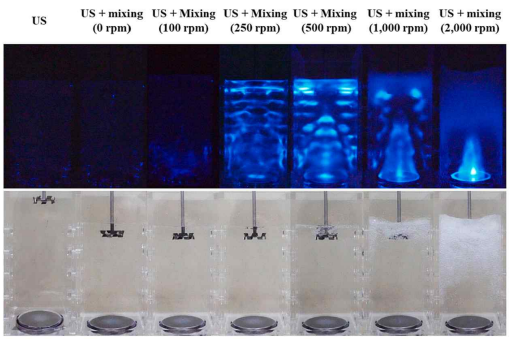
Ultrasonics Sonochemistry
Volume 101, December 2023, 106659 (Impact Factor : 8.4)

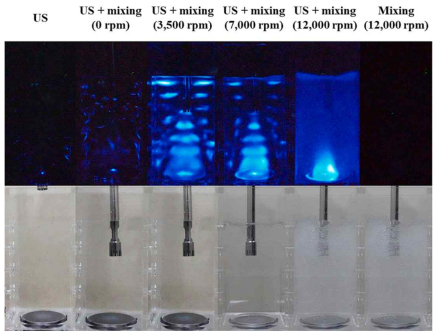
Effect of violent mixing on sonochemical oxidation activity under various geometric conditions in 28-kHz sonoreactor

Dukyoung Lee, Jumin Kang, Younggyu Son









The effects of violent mixing and reactor geometric conditions were investigated using the overhead stirrer and high-speed homogenizer in 28-kHz sonoreactors. The sonochemical oxidation activity was quantified using the KI dosimetry method, and the sonochemical active zone was visually observed using the luminol method. Higher mixing rates resulted in a significant enhancement of the sonochemical oxidation activity, primarily due to a significant change in the sonochemical active zone. When using the overhead stirrer (0–2,000 rpm), the highest activity for 2λ and 3λ occurred at 500 rpm, whereas the highest activity for 4λ was obtained at 250 rpm. For the high-speed homogenizer (0–12,000 rpm), the highest activity was consistently obtained at 3,500 rpm across all liquid height conditions. The impact of mixing position (Top, Mid, and Bot positions) on sonochemical activity was analyzed. The results revealed that the lowest activity was obtained for the bottom position, likely attributed to significant ultrasound attenuation. The reactor size effect was investigated using the high-speed homogenizer in five cylindrical sonoreactors with different diameters (12–27 cm). It was found that very low activity could be observed due to unexpected geometric conditions, and the application of mixing (3,500 rpm in this study) could result in high sonochemical activity regardless of geometric conditions.