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KIT Energy News

에너지융합기술 혁신인재 양성사업단

Innovative Education & Research Center for Energy Convergence Science and Technology

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KIT Energy 소식

신소재공학부 박철민 교수 연구팀, '신개념 리튬화합물 음극 소재' 개발

- 높은 초기 효율과 안정성 동시 충족, 새로운 분류의 리튬이차전지 음극 제안
- 차세대 고성능 이차전지 음극 소재로서 상용화 가능성 높아



신소재공학부 전지신소재연구실(Advanced Battery Materials Lab.) 박철민 교수 연구팀이 '고성능 리튬이차전지용 신개념 리튬화합물 음극 소재' 개발에 성공했다.

박철민 교수 연구팀은 최근 신개념 음극 소재로 분류될 것으로 기대되는 다양한 리튬화합물(Li-compound)을 제조한 데 이어, 이를 리튬이차전지용 음극 소재로 적용하여 전지 성능의 우수성을 확인했다.

고용량의 이차전지를 구현하기 위해서는 이온용량이 높은 리튬 금속 및 실리콘을 음극 소재로 사용해야 하지만, 현재 상용화되고 있는 흑연 음극 소재는 제한적 용량(372 mAh/g)으로 인해 고용량 이차전지를 구현하는 데 어려움이 있다.

리튬 금속은 금속 자체의 높은 반응성으로 인해 안전성에 대한 우려가 있고, 실리콘 음극은 충전 및 방전 시 수명이 저하되는 한계를 가진다. 또한, 이러한 음극들은 초기 충전 시 일정량의 리튬이온이 영구 손실되는 문제도 있다.

영구 손실되는 리튬이온은 이차전지 가격에서 가장 큰 비중을 차지하는 양극에서 제공되기 때문에 초기 손실을 줄이고, 초기 효율을 향상시킬 수 있는 관련 기술이 다양하게 연구되고 있는 상황이다.

현재 알려진 초기효율을 향상시킬 수 있는 대표적인 방법은 리튬을 음극 소재에 미리 저장시키는 '사전리튬화(pre-lithiation)' 기술이다. 하지만, 사전리튬화 기술은 복잡한 공정 및 제어가 요구되며, 사전리튬화 처리된 소재는 대기 중에서 높은 반응성을 보이기 때문에 실제 상용화 단계에 도달하기에는 많은 어려움이 있다.

이러한 기존 음극 소재의 한계를 극복하기 위해, 박철민 교수 연구팀은 다양한 '리튬화합물 음극 소재' 개념을 새롭게 제안했다. 리튬화합물 음극 소재는 기존 상용화된 음극 소재들과 비교하여 더 높은 초기 효율과 용량, 그리고 출력 특성을 보였다. 또한, 리튬화합물 음극은 일반적인 대기 중에서도 높은 안정성을 보인 점이 주목할 만하다.

그동안 다양한 이차전지 시스템과 고용량 전극 소재 개발 등 차세대 산업 동력을 위한 연구를 지속적으로 이어오고 있는 박철민 교수는 "이번 성과는 리튬이차전지는 리튬을 포함하는 양극소재 및 리튬을 포함하지 않는 음극소재로 구성된다는 기존 사고의 틀을 벗어나는 것으로, 이차전지 전극 소재 관련 연구에 새로운 패러다임을 제시할 것이며, 고성능 음극 소재의 실질적 상용화에도 크게 기여할 수 있을 것으로 기대된다"고 말했다.

4단계 BK21사업, 중견연구자지원사업 및 우리 대학 Grand-ICT연구센터사업 지원으로 수행된 이번 연구는 우리 대학 BK21 에너지융합기술 혁신인재 양성사업단 남기훈 박사후 연구원이 제1저자로 참여했으며, 인하대 환경공학과 전기준 교수 및 정상민 박사후 연구원, 한국전기연구원 최정희 박사, 미국 전기차 업체 리비안(Rivian) 유병철 박사와의 공동 연구로 진행됐다.

관련 연구는 나노소재분야 세계적 권위지 'ACS Nano(IF=18.027)' 온라인판에 9월 27일자로 게재됐으며, 연구 결과의 중요성을 인정받아 표지논문으로 선정되는 쾌거를 거뒀다. 또한 관련 특허 2건도 출원했다.

금오공과대학교 KIT People(2022.10.04.) https://www.kumoh.ac.kr/ko/sub01_05_02.do?mode=view&articleNo=408867

◆ 관련 기사 ◆

연합뉴스	금오공대, 차세대 고성능 이차전지 음극 소재 개발	https://www.vna.co.kr/view/AKR20221004129600053
뉴데일리	국립금오공대 박철민 교수 연구팀, '신개념 리튬화합물 음극 소재' 개발	https://tk.newdaily.co.kr/site/data/html/2022/10/04/2022100400272.html
뉴시스	금오공대, 차세대 이차전지 리튬화합물 음극 소재 개발	https://newsis.com/view/?id=NISX20221005_0002037231
대구일보	고성능 리튬이차전지용 리튬화합물 음극 소재 개발...금오공대 박철민 교수 연구팀	http://www.idaegu.com/newsView/idg202210040080
경북일보	금오공대 박철민 교수 연구팀, 이차전지용 신개념 리튬화합물 음극소재 개발	http://www.kyongbuk.co.kr/news/articleView.html?idxno=2113521
경북도민일보	국립금오공대, 박철민 교수 연구팀...고성능 리튬이차전지용 '신개념 리튬화합물 음극 소재' 개발	http://www.hidomin.com/news/articleView.html?idxno=495487
브레이크뉴스	금오공대, 신개념 리튬화합물 음극 소재 개발 성공	https://www.breaknews.com/928410
매일신문	구미 금오공대 박철민 교수 연구팀, '신개념 리튬화합물 음극 소재' 개발	https://news.imaeil.com/page/view/2022100415422725943
한국대학신문	금오공대 박철민 교수팀, 고성능 리튬이차전지용 '신개념 리튬화합물 음극 소재' 개발	https://news.unn.net/news/articleView.html?idxno=534881
전자신문	금오공대, 고성능 리튬이차전지용 신개념 리튬화합물 음극 소재 개발	https://www.etnews.com/20221004000260
서울경제	이차전지용 신개념 리튬화합물 음극소재 개발	https://www.sedaily.com/NewsView/26C7X9DQSG
교수신문	국립금오공대, 박철민 교수 연구팀 고성능 리튬이차전지용 '신개념 리튬화합물 음극 소재' 개발	http://www.kyosu.net/news/articleView.html?idxno=94829
데일리한국	금오공대 박철민 교수 연구팀, 고성능 리튬이차전지용 '신개념 리튬화합물 음극 소재' 개발	https://daily.hankooki.com/news/articleView.html?idxno=878407

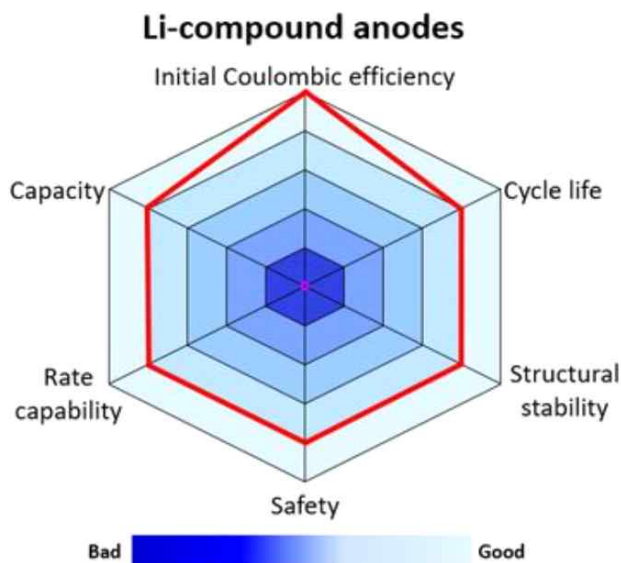
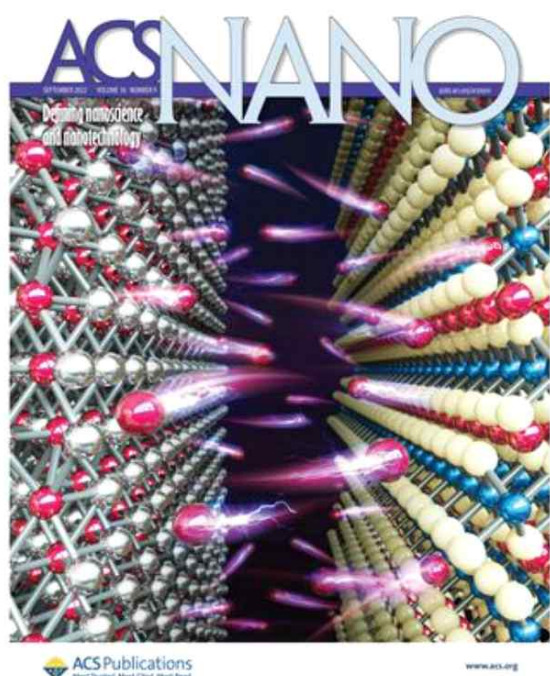
에너지저장

ACS Nano

Volume 16, September 2022, p13704-13714 (Impact Factor : 18.027)

Li-Compound Anodes: A Classification for High-Performance Li-Ion Battery Anodes

Ki-Hun Nam, Sangmin Jeong, Byeong-Chul Yu, Jeong-Hee Choi, Ki-Joon Jeon*,
and Cheol-Min Park*



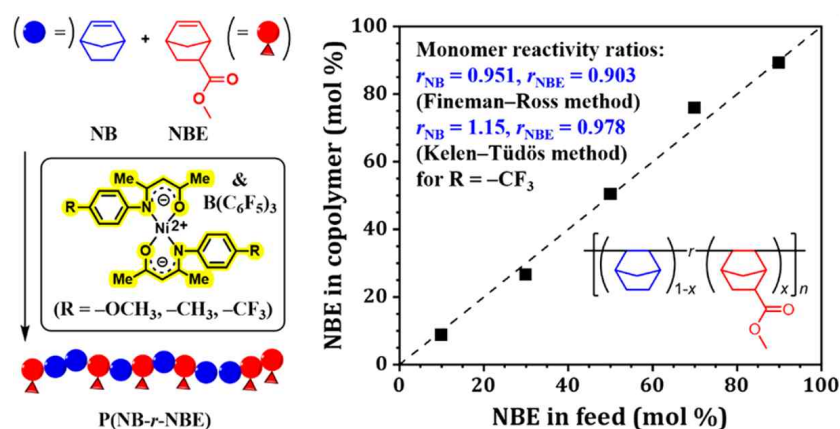
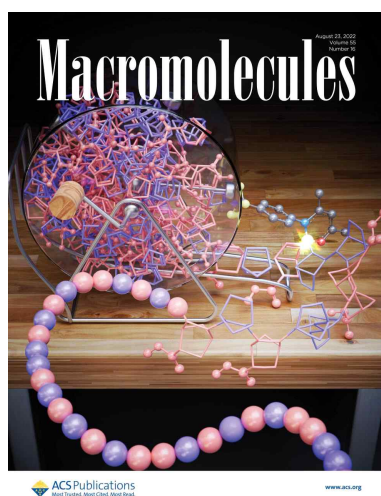
Four main anode types are generally considered as typical anodes for Li-ion batteries (LIBs): Li-metal, carbon-based, alloy-based, and oxide-based anodes. Although they exhibit satisfactory electrochemical performance as LIB anodes, they cannot simultaneously satisfy all key requirements for LIB anodes: high reversible capacity, high initial Coulombic efficiency (ICE), long cycle life, fast rate capability, structural stability, and no safety concerns. Here, we suggest Li-compound anodes as a promising class of high-performance LIB anodes. Three binary (LiSn , Li_2Sb , and LiBi) and three ternary (Li_2ZnSb , Li_5GeP_3 , and Li_5SnP_3) Li compounds were introduced as Li-compound anodes. LiSn and Li_5SnP_3 were selected and further modified into their nanocomposites by solid-state synthetic routes using carbon sources for high-performance LIB anodes. The Li-compound nanocomposite anodes exhibited excellent performance and simultaneously fulfilled all the key requirements for high-performance LIB anodes. Therefore, Li-compound anodes are expected to be a promising and innovative category of high-performance LIB anodes.

Macromolecules

Volume 55, August 2022 p.7049–7058 (Impact Factor : 6.057)

Bis(β-ketoimino)nickel(II) Complexes for Random Copolymerization of Norbornene and Methyl 5-Norbornene-2-carboxylate with Controlled Ester Group Incorporation

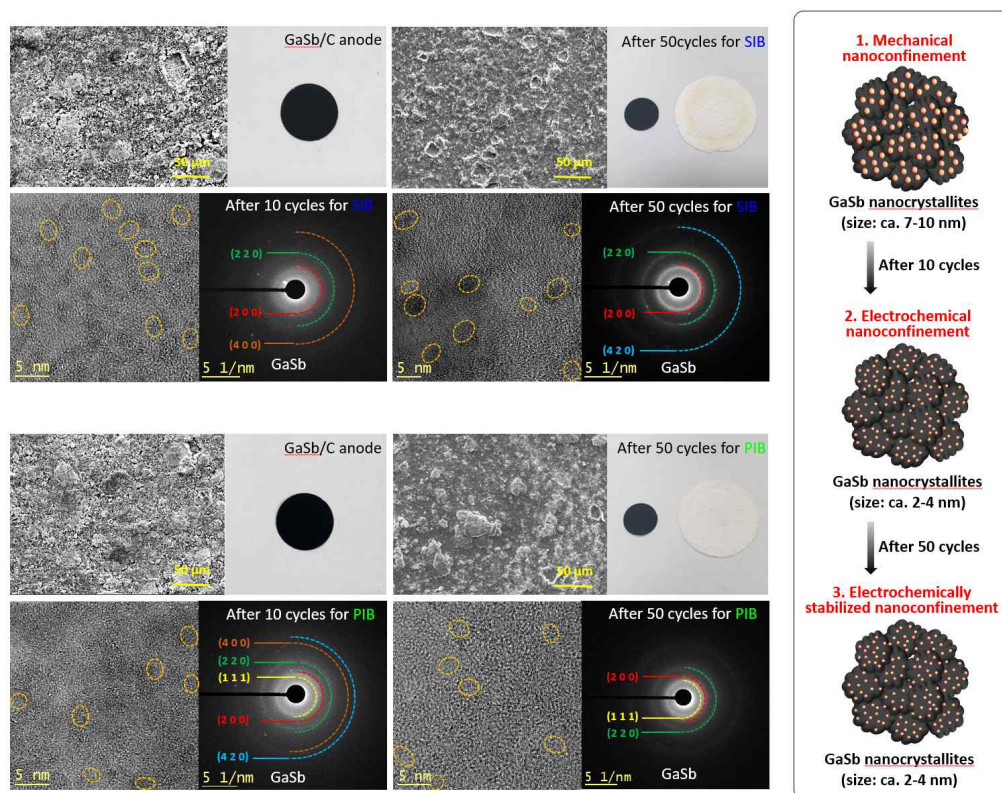
Chang-Geun Chae, Jun Woo Park, Linh N. T. Ho, Myung-Jin Kim, Eun Chae Kim, Woohwa Lee, Sungmin Park, Dong-Gyun Kim*, Hyun Min Jung*, and Yong Seok Kim*



A series of bis(β-ketoimino)nickel(II) complexes with *p*-substituted *N*-phenyl groups, Ni[CH₃C(O)CHC(NPhR)-CH₃]₂ (Ni1: R = -OCH₃; Ni2: R = -CH₃; Ni3: R = -CF₃), were synthesized, and their general coordination geometry was elucidated by single-crystal X-ray diffraction analysis of Ni3. These complexes were paired with tris(pentafluorophenyl)borane (B(C₆F₅)₃) to catalyze the vinyl addition copolymerization of norbornene (NB) and methyl 5-norbornene-2-carboxylate (NBE). All the catalyst systems exhibited high catalytic activities ($>10^5$ g_{polymer} mol_{Ni}⁻¹ h⁻¹) at NBE feed contents of up to 50 mol %, resulting in the production of copolymers with high molecular weights ($M_w = 135 - 355$ kg mol⁻¹, $\bar{D} = 1.78 - 2.12$). In addition, the content of polar ester groups was precisely controlled by the feed ratio of the monomers. For Ni3, two monomer reactivity ratios were found to be close to unity (Fineman-Ross method: $r_{NB} = 0.951$, $r_{NBE} = 0.903$; Kelen-Tüdös method: $r_{NB} = 1.15$, $r_{NBE} = 0.978$). Since the copolymerization behaviors were revealed to be independent of the electronegativity of *p*-substituent, all the catalyst systems of Ni1-Ni3/B(C₆F₅)₃ were considered to serve the random copolymerization of NB and NBE. The resulting poly(norbornene-*random*-methyl 5-norbornene-2-carboxylate)s exhibited the dielectric and surface properties well tunable by compositional modulation.

GaSb nanocomposite: New high-performance anode material for Na- and K-ion batteries

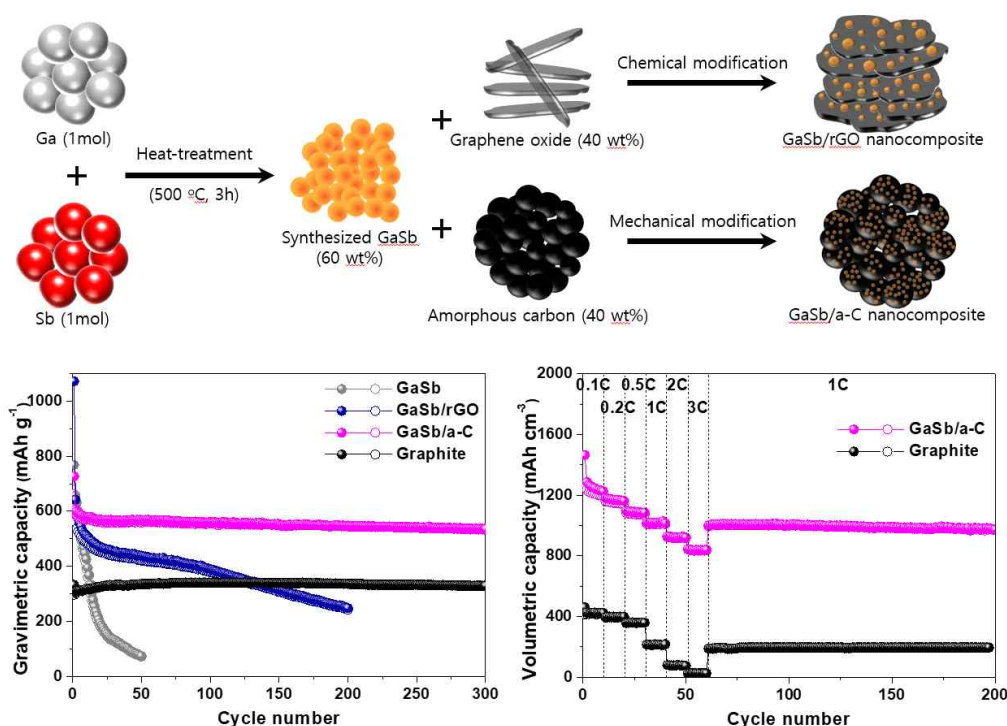
KIn-Su Hwang, Young-Han Lee, Jeong-Myeong Yoon, Yoon Hwa*, Cheol-MinPark*



As representative next-generation secondary battery systems, sodium-ion batteries (SIBs) and potassium-ion batteries (PIBs) are key candidates to achieve zero-carbon emission. Herein, we introduce a versatile GaSb nanocomposite anode for SIBs and PIBs. The performance and phase transition mechanism for GaSb, pure Ga, and Sb with Na and K ions are evaluated. Furthermore, three-step nanoconfinement and stabilization of GaSb crystallites are achieved in the GaSb nanocomposite. The nanostructure of the GaSb nanocomposite, consisting of approximately 2-4 nm GaSb crystallites uniformly distributed in an amorphous carbon matrix, promotes the electrochemical reaction kinetics with Na and K ions, and the chemical and mechanical stabilities of the GaSb nanocomposite electrodes. The GaSb nanocomposite anode possesses highly reversible initial volumetric and gravimetric capacities and superior high-rate capabilities. In this study, we offer new insights into the phase transition mechanisms of GaSb with Na and K ions and promising performance GaSb nanocomposite anodes for SIBs and PIBs.

High-Energy-Density Gallium Antimonide Compound Anode and Optimized Nanocomposite Fabrication Route for Li-Ion Batteries

In-Su Hwang, Young-Han Lee, Vinoth Ganesan, Yoon Hwa*, and Cheol-Min Park*



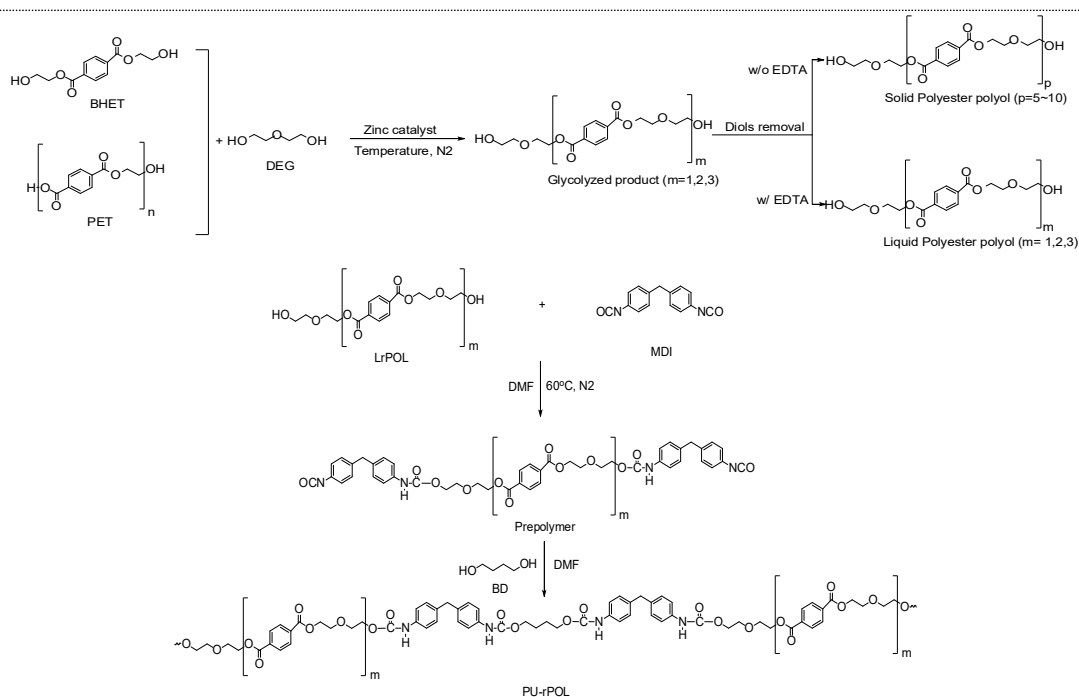
Lithium-ion batteries (LIBs) are key enablers for achieving net-zero emission by transitioning from fossil fuels to renewable energy. This study introduces a GaSb compound anode and optimized nanocomposite fabrication route for superior LIBs. First, to utilize the synergistic effect of Ga and Sb, their GaSb compound was synthesized using a simple thermal solid-state reaction. Furthermore, the anode performance and reaction mechanisms of GaSb and elemental Ga and Sb with Li ions are demonstrated fully using cutting-edge analysis tools. Second, two nanocomposite fabrication routes are suggested to obtain optimized GaSb anodes for LIBs: (1) reduced graphene oxide (rGO)-decorated GaSb nanocomposite (GaSb/rGO) by a chemical modification and (2) amorphous C (a-C)-decorated GaSb nanocomposite (GaSb/a-C) by a mechanical modification. Among the nanocomposites, the GaSb/a-C shows better electrochemical performance, achieved by the three-step nanoconfinement and stabilization of tiny GaSb crystallites (approximately 2–4 nm) homogeneously embedded in the carbon matrix. The proposed GaSb/a-C anode exhibits highly reversible gravimetric/volumetric capacities, long-term cyclability, and excellent high rate capabilities, which are much better than conventional graphite anodes. In this study, we provide an insight into the reaction mechanism of GaSb with Li ions and suggest a high-energy-density GaSb compound anode for LIBs.

Polymer Degradation and Stability

Volume 205, November 2022, p.110147 (Impact Factor : 5.204)

Direct conversion of waste polyesters to low molecular weight polyols for polyurethane production

Dieu Minh Ngo, Kyunghan Lee, Linh Nguyet Thi Ho, Jinseok Lee, Hyun Min Jung*



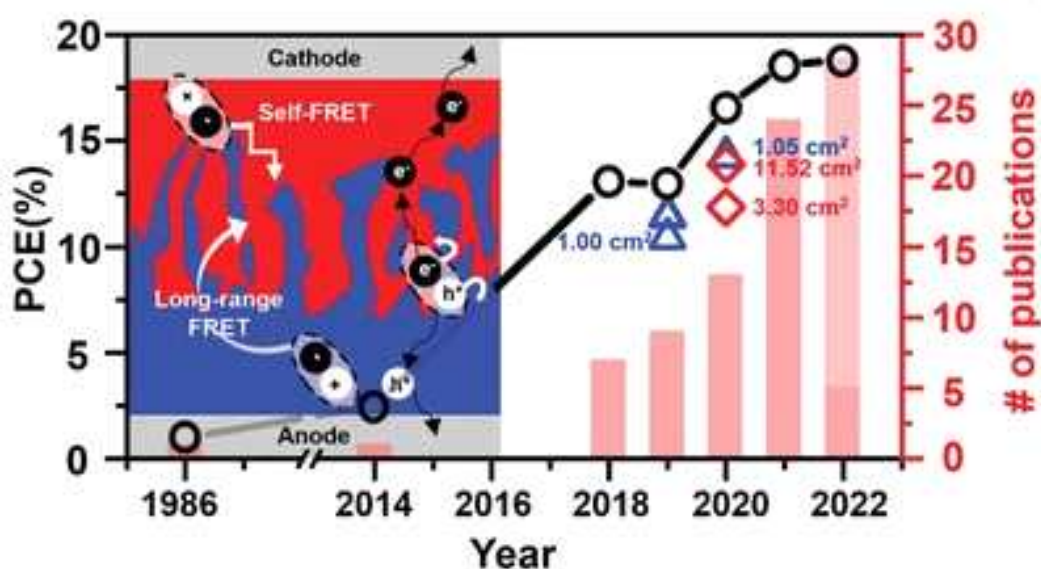
An effective process for synthesizing liquid dihydroxyl group-ended oligomers directly from waste polyethylene terephthalate (PET) using a metal chelating agent, ethylenediaminetetraacetic acid (EDTA), is described in this study. The deactivation of transesterification catalyst was confirmed by a model process that involves the re- action of bis(2-hydroxyethyl) terephthalate with diethylene glycol under different catalytic conditions. The depolymerization of PET was performed with an excess amount of diethylene glycol and Zn²⁺ catalysts to form intermediates. The chelating agent was then introduced as a catalytic defunctionalizer, after which the residual glycols were distilled and recovered under reduced pressure. The obtained polyols were characterized by ¹H and ¹³C nuclear magnetic resonance, gel permeation chromatography, and viscometry. Utilizing EDTA showed high efficiency in blocking catalysts during high-temperature distillation, resulting in maximum trimer chain-length sized and low-viscosity liquid polyols. Subsequently, thermoplastic polyurethanes (TPUs) were prepared using synthesized polyols as the soft segment, with 4,4'-methylene-bis(phenyl isocyanate) and 1,4-butanediol as the isocyanate and chain extender, respectively. The final TPUs were characterized using Fourier-transform infrared spectroscopy, thermogravimetric analysis, and mechanical testing.

Advanced Science

Volume 9, September 2022, p2201876 (Impact Factor : 17.521)

Recent Advances in Nonfullerene Acceptor-Based Layer-by-Layer Organic Solar Cells Using a Solution Process

Min Hun Jee, Hwa Sook Ryu, Dongmin Lee, Wonho Lee*, Han Young Woo*



Recently, sequential layer-by-layer (LbL) organic solar cells (OSCs) have attracted significant attention owing to their favorable p-i-n vertical phase separation, efficient charge transport/extraction, and potential for lab-to-fab large-scale production, achieving high power conversion efficiencies (PCEs) of over 18%. This review first summarizes recent studies on various approaches to obtain ideal vertical D/A phase separation in nonfullerene acceptor (NFAs)-based LbL OSCs by proper solvent selection, processing additives, protecting solvent treatment, ternary blends, etc. Additionally, the longer exciton diffusion length of NFAs compared with fullerene derivatives, which provides a new scope for further improvement in the performance of LbL OSCs, is discussed. Large-area device/module production by LbL techniques and device stability issues, including thermal and mechanical stability, are also reviewed. Finally, the current challenges and prospects for further progress toward their eventual commercialization are discussed.

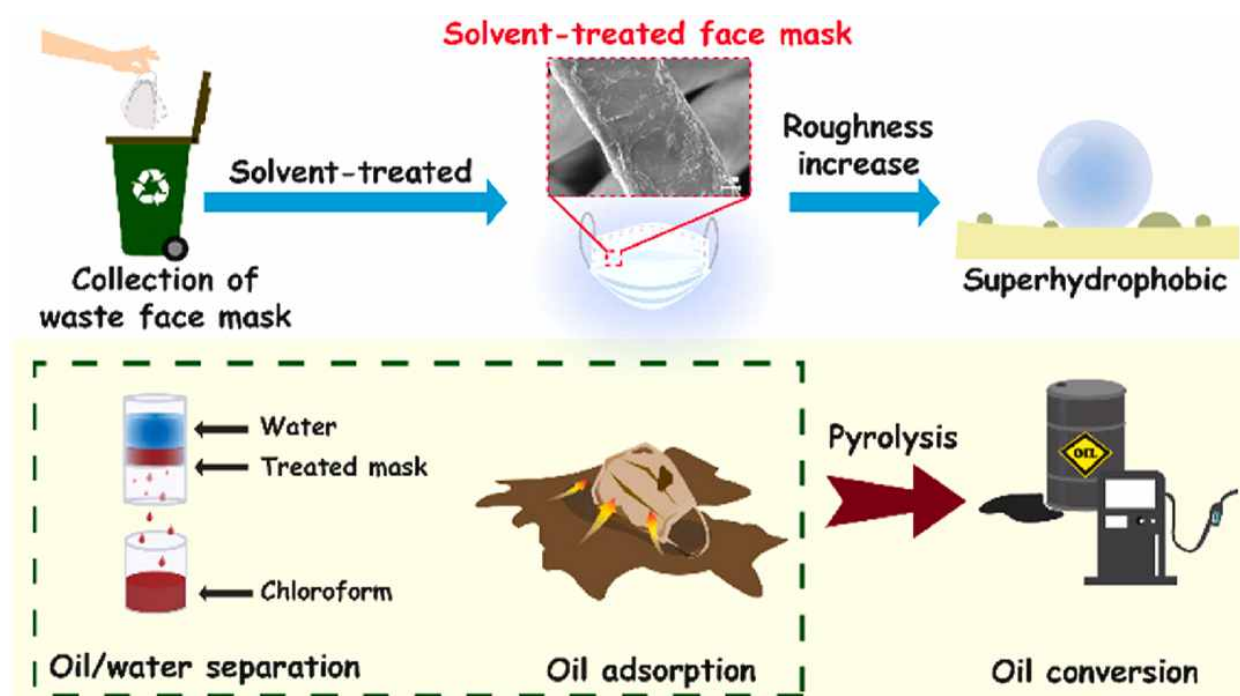
환경에너지

Chemosphere

Volume 303, September 2022, p135186 (Impact Factor : 8.943)

Superhydrophobic polypropylene sorbent derived from discarded face masks: A highly efficient adsorbent for oil spill sorbent

Sejin Park, Yoonho Kim, Wonho Lee*, Changwoo Nam*



Globally, an estimated 130 billion face masks are used and disposed of every month. Thus, recycling or upcycling discarded face masks has attracted significant attention due to economic benefits and environmental concerns. To reduce the amount of used face masks going to waste, this study features a superhydrophobic face mask prepared by simple chemical modification with environmentally preferable alkane solvents (n-hexane, n-heptane, and n-decane), that is effective as a sorbent for oil spill cleanup. All alkanes examined increased the surface roughness of the face masks and improved face mask hydrophobicity. The heptane treated face mask (at 90 °C for 1 h), can adsorbed Arabian light crude oil up to 21 times of their weight on the water surface. In addition, chloroform, toluene, gasoline, and diesel were adsorbed 18, 13, 8 and 16 times, respectively. More importantly, heptane has a high recycling efficiency as a treatment solvent and is reusable for at least 10 cycles of mask surface treatment. Consequently, this inexpensive and easily fabricated material is a promising development in waste face mask (WFM) upcycling.