

ReaxysAI Search 및 Prediction Retrosynthesis

ReaxysAI는 Reaxys데이터를 기반으로 하여 1억 2,100만 개 이상의 문서 (특허 및 검증된 학술논문)에 접근할 수 있으며, 높은 정밀도와 재현성을 갖춘 답변을 제공합니다. 수백명의 다양한 분야의 화학자들과의 테스트 과정을 거쳐 개발 되었으며, 자연어 검색을 통해 분야와 경험 수준에 상관없이 연구자들이 신뢰성 있는 데이터의 정보를 더 빠르게 찾을 수 있도록 지원합니다. 또한, 지속적으로 피드백을 수집하여 검색 옵션의 추가 개선과 고급 요약 기능도 업데이트 할 예정입니다.

최신 AI 중심의 Reaxys를 통해 화학을 중심으로 하는 연구, 개발, 교육의 혁신을 함께 이뤄가겠습니다.

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Benefits of using Single-Crystal Cathode Particles in lithium-ion batteries

100+ Documents found

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검색 결과의 문헌들에 대한 필터 및 구조화된 데이터 검색 가능

1 **Single-crystal high-nickel layered cathodes for lithium-ion batteries: advantages, mechanism, challenges and approaches** [2022]
Score: 0.999707

Abstract:
The ever-increasing demand of advanced lithium-ion batteries is calling for high-performance cathode materials. Among promising next-generation cathode materials, high-nickel layered oxides with spherical polycrystalline secondary particles exhibit the outstanding advantage of high energy density. However, polycrystals, suffered from the pulverization of particles and the expansion of cracks, show the shortcoming of poor cycling performance. As an efficient solution, the single-crystal route has been underestimated hitherto. Herein, the unique structural degradation mechanism of single crystals is emphasized, and their advantages against polycrystals are comprehensively summarized in terms of electrochemical, thermal, and mechanical properties. Furthermore, we point out the practical challenges of single-crystal materials toward practical applications and raise hopeful strategies for overcoming such issues. Based on the aforementioned characteristics and approaches, future directions are outlooked as well.

Was this relevant to the question? ☐ ☐

2 **Pulse High Temperature Sintering to Prepare Single-Crystal High Nickel Oxide Cathodes with Enhanced Electrochemical Performance** [2023]
Score: 0.999528

Abstract:
For the currently most dominant cathode of $\text{Li}(\text{Ni}_{1-x}\text{Co}_x\text{Mn}_x\text{O}_2)$ (NCM, $x+y+z=1$) in lithium-ion batteries, higher nickel content brings higher energy density but is accompanied by heavier interfacial reactions with electrolyte and worse safety performance. Single crystal cathode materials have the advantages of fewer grain boundaries, higher density, and greatly suppressed microcracks during cycling, these benefits in turn suppress interfacial side reactions, as well as the improve volumetric energy density and safety performance. Here, a strategy of pulse high-temperature sintering (PHTS) is reported to prepare single-crystal $\text{Li}(\text{Ni}_{0.9}\text{Co}_{0.05}\text{Mn}_{0.05}\text{O}_2)$ (SC-NCM90), in which an extra PHTS at 1040°C for 1 min is added in the traditional calcination process at 750°C , yielding well defined octahedral particles with an initial capacity of 209 mAh g⁻¹. Compared with the counterpart NCM90 secondary spheres, the tap density of SC-NCM90 increases by 1/3 to 2.76 g cm⁻³ and the microcracks are successfully suppressed, improving both the cycling performance and thermal stability. The calcination time and temperature are optimized, showing that overlong time or overhigh temperature of the PHTS treatment would result in particles with better defined octahedral shape but heavier Li/Ni intermixing and capacity loss.

Was this relevant to the question? ☐ ☐

Predictive Retrosynthesis:

최신 IKTOS사의 예측모델을 통해 합성라이브러리 전략을 다양하게 구축해보세요!
합성전략의 다양한 아이디어를 나만의 것으로!!!

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Structure editor selected: MarvinJS ChemDrawJS

Insert structure from name > Parameters

Predicted ☒ **Published** ☐

20 full routes (up to 10)
3 identical reaction steps per project (up to 10)
3 identical building blocks per project (up to 10)
10 min processing time
Rx STD SML LNK EM US G2 T3 building block

Full routes (up to 10)
branches per route (up to 10)
steps per route (up to 10)
Don't stop at commercial building blocks
% yield per step (assumed, if not published)

Length of routes ☒ Max. Number of steps: 15 (2-15) ☐ First disconnect only

Stereo and Regioselectivity ☐ Ignore stereochemistry ☐ Only regioselective reactions

Starting materials settings **Reaxys Commercial Substances (RCS)**

Max. Shipping time ☐ up to 10 days ☒ any

Max. Price per gram: any (\$/g)

Processing time ☒ Standard ☐ Extended

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