



Záverečná karta projektu

Názov projektu

Evidenčné číslo projektu

APVV-19-0465

Hybridné nízkorozmerné vrstevnaté materiály s novými funkciami

Zodpovedný riešiteľ **Ing. Mária Omastová, DrSc.**

Príjemca **Ústav polymérov SAV, v. v. i.**

Názov pracoviska, na ktorom bol projekt riešený

Hlavný riešiteľ: Ústav polymérov SAV, v.v.i.

Spoluriešiteľ: Fyzikálny ústav SAV, v. v. i.

Názov a štát zahraničného pracoviska, ktoré spolupracovalo pri riešení

Udelené patenty/podané patentové prihlášky, vynálezy alebo úžitkové vzory, ktoré sú výsledkami projektu

Najvýznamnejšie publikácie (knihy, články, prednášky, správy a pod.) zhrňujúce výsledky projektu – uveďte aj publikácie prijaté do tlače

Publikácie v zahraničných karentovaných časopisoch
2021

1. ALI, Israt - DIN, Muhammad Faraz Ud - KÁLOSI, Anna - ANNUŠOVÁ, Adriana - LABUDOVA, Martina - JERGEL, Matej - SOYKA, Yaryna - OMASTOVÁ, Mária - MAJKOVÁ, Eva. Facile fabrication of Ti3C2 MXene nanosheets and their photothermal properties. In NANOCON 2021 Proceedins 13th International Conference on Nanomaterials - Research & Application, October 20-22, 2021, Brno, Czech Republic. - Ostrava, Czech Republic, pg. 258-264, ISBN: 978-80-88365-00-6, DOI: <https://doi.org/10.37904/nanocon.2021.4359>, Typ: ADMB

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3. MACHATA, Peter et al.. An In-depth study of the wettability of MXene films. In The 6th International conference on nanomaterials: Fundamentals and applications: Book of abstracts. Košice, 16.-19.10.2022. - Košice: Prírodovedecká fakulta UPJŠ, 2022, p. 99-100. ISBN 978-80-5740127-8. (International conference on nanomaterials: Fundamentals and applications.)
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Uplatnenie výsledkov projektu

Príprava perovskitových solárnych článkov (PSC), vrátane použitia nanoštrukturovaných materiálov typu 0D a 2D, je rozhodujúcim faktorom pre budúci vývoj nových typov solárnych článkov so zlepšenými vlastnosťami, maximálnou účinnosťou pri minimálnej hmotnosti a rozmeroch. Dosiahnuté výsledky projektu otvárajú možnosti pre nové kreatívne riešenia pre zvyšovanie efektívnosti konverzie solárnej energie na elektrickú energiu nových typov solárnych článkov na báze perovskitov a MXénových nanomateriálov.

Súhrn výsledkov riešenia projektu a naplnenia cieľov projektu v slovenskom jazyku (max. 20 riadkov)

Projekt riešil aktuálne problémy v oblasti výskumu aplikácie 2D materiálov, MXénov, perovskitových kvantových bodiek a ich zabudovania v inovatívnych perovskitových

fotovoltických a optoelektronických štruktúrach. MXény nie sú komerčne dostupné v potrebnej kvalite, preto sa pripravili vo forme delaminovaných monovrstiev z MAX fáz. Na začiatku projektu sa pripravil MXén typu M3X2 - Ti3C2 Tx, v neskorších štádiách výskumu to bol typ M4C3 - V4C3.

Perovskitové kvantové bodky (PQDs) typ CsPbX3 (X = halogenid) boli pripravené v prvej fáze ako CsPbI3, a neskôr ako CsPbBr3 a stabilizované rôznymi ligandami. V ďalšom štádiu sa pripravili jednotlivé kompaktné a usporiadané monovrstvy MXénových častíc a PQDs na rozhraní voda/vzduch modifikovanou Langmuir-Schaefer metódou.

Skúmal sa vplyv modifikácie Ti3C2Tx MXénu na transportnú vrstvu elektrónov SnO2 (ETL) pre koncentračný rozsah 0–7,4 hm. % MXénu. Zo získaných údajov vyplýva, že pridaný MXén zlepšuje transport elektrónov, čo priamo súvisí s jeho takmer kovovým správaním. Výsledky ER-EIS naznačujú, že prídavok do 1 hm. % MXénu v SnO2 ETL je ešte akceptovateľný, aby si ETL zachovala povahu blokovania dier, zatiaľ čo pri vyššej koncentrácii sa táto vlastnosť stráca. Účinok MXénu na štruktúru a morfológiu ETL perovskitovej vrstvy sa pozoroval pomocou SEM a in situ GIWAXS. Potvrdila sa zvýšená veľkosť perovskitových zŕn na SnO2 ETL modifikovanej MXénom v porovnaní s čistou SnO2 ETL. Počas žihania bol pomocou in situ GIWAXS pozorovaný rastúci počet zŕn. Tieto výsledky sú interpretované pomocou modelu nukleácie a rastu. Zvýšená účinnosť konverzie energie zo 17,4 % na 18,3 % metylamónium-olovo-jodidového perovskitového solárneho článku po modifikácii SnO2 ETL s 0,1 hm.% MXénu je výsledkom dvoch príspevkov (i) zvýšenej elektrickej vodivosti modifikovanej ETL a (ii) zlepšenej kryštalinity a väčšej veľkosti perovskitových zŕn v porovnaní s perovskitovou vrstvou rastenou na čistej SnO2 ETL, čo znižuje celkovú hraničnú plochu a rekombináciu náboja na defektných stavoch (pasciach), ktoré sa typicky tvoria na hraniciach zŕn.

Súhrn výsledkov riešenia projektu a naplnenia cieľov projektu v anglickom jazyku (max. 20 riadkov)

The project solved current problems in the field of research on the application of 2D materials, MXenes, perovskite quantum dots and their incorporation into innovative perovskite photovoltaic and optoelectronic structures. MXenes are not commercially available in the required quality, therefore they were prepared in the form of delaminated monolayers from MAX phases. At the beginning of the project, MXene type M3X2 - Ti3C2Tx was prepared, in the later stages of the research it was the type M4C3 - V4C3.

Perovskite quantum dots (PQDs) type CsPbX3 (X = halide) were prepared in the first stage as CsPbI3, and later as CsPbBr3, and stabilized by different ligands. In the next project phase, individual compact and ordered monolayers of MXene particles and PQDs were prepared at the water/air interface by the modified Langmuir-Schaefer method.

The influence of the Ti3C2Tx MXene modification on the SnO2 electron transport layer (ETL) was investigated in the concentration range 0–7.4 wt.% of MXene. The obtained data showed that added MXene improves electron transport, which is directly related to its almost metallic behavior. The ER-EIS results indicate that the addition of up to 1 wt. % of MXene in SnO2 ETL is still acceptable for the ETL to retain the hole-blocking nature, while at higher concentration this property is lost. The effect of MXene on the structure and morphology of the ETL perovskite layer was observed by SEM and in situ GIWAXS.

An increased size of perovskite grains on MXene modified SnO2 ETL compared to pure SnO2 ETL was confirmed. During annealing, an increasing number of grains was observed by in situ GIWAXS. These results are interpreted using a nucleation and growth model. The increased power conversion efficiency from 17.4 % to 18.3 % of the methylammonium-lead-iodide perovskite solar cell after modification of the SnO2 ETL with 0.1 wt% MXene is the result of two contributions (i) the increased electrical conductivity of the modified ETL and (ii) the improved crystallinity and larger perovskite grain size compared to a perovskite layer grown on pure SnO2 ETL, which reduces the total interfacial area and charge recombination on defect states (traps) that typically form at grain boundaries.