

**POLIMERLAR KIMYOSI VA FIZIKASI INSTITUTI
HUZURIDAGI ILMIY DARAJALAR BERUVCHI
DSc.02/30.12.2019.K/FM/T.36.01 RAQAMLI ILMIY KENGASH
ASOSIDAGI BIR MARTALIK ILMIY KENGASH**

POLIMERLAR KIMYOSI VA FIZIKASI INSTITUTI

JO'LLIYEV ZAVQIDDIN NORMENGLI O'G'LI

**PEROVSKIT YUTUVCHI QATLAMINING SHAKILLANISH
XUSUSIYATLARI BILAN UNGA ASOSLANGAN QUYOSH
ELEMENTLARINING KONVERSIYA KO'RSATKICHLARI O'RTASIDAGI
BOG'LIQLIK**

**01.04.06 – Polimerlar fizikasi
02.00.12 – Nanokimyo, nanofizika va nanotexnologiya**

**FIZIKA - MATEMATIKA FANLARI BO'YICHA FALSAFA DOKTORI (PhD)
DISSERTATSIYASI AVTOREFERATI**

Toshkent – 2025

**Fizika - matematika fanlari bo‘yicha falsafa (PhD) doktori
dissertatsiyasi avtoreferati mundarijasi**

**Оглавление автореферата диссертации доктора философии (PhD)
физико – математическим наукам**

**Contents of dissertation abstract of doctor of philosophy (PhD) on Physics and
Mathematics sciences**

Jo‘llyev Zavqiddin Normengli o‘g‘li

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Fizika - matematika fanlari bo'yicha falsafa doktori (PhD) dissertatsiyasi mavzusi O'zbekiston Respublikasi Vazirlar Mahkamasi huzuridagi Oliy attestatsiya komissiyasida B2025.2.PhD/FM1331 raqam bilan ro'yxatga olingan.

Dissertatsiya Polimerlar kimyosi va fizikasi institutida bajarilgan.

Dissertatsiya avtoreferati uch tilda (o'zbek, rus, ingliz (rezyume)) Ilmiy kengash veb-sahifasida (polchemphys.uz) va «Ziyonet» axborot-ta'lim portalida (www.ziyonet.uz) joylashtirilgan.

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Dissertatsiya avtoreferati 2025 yil «__» **dekabr** kuni tarqatildi.
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KIRISH (falsafa doktori (PhD) dissertatsiyasi annotatsiyasi)

Dissertatsiya mavzusining dolzarbligi va zarurati. Dunyoda aholi soni o‘sib borayotgani sababli energetik resurslarga bo‘lgan talab global miqyosda shiddat bilan oshmoqda. Bu yo‘nalishda, arzon, ishlab chiqarish texnologiyasi sodda va yuqori samaradorlikka ega perovskit quyosh elementlarini yaratish dolzarb muammolardan biri hisoblanadi.

Bugungi kunda jahonning yetakchi ilmiy markazlarida perovskit asosidagi quyosh elementlarida yuqori samaradorlikka erishish uchun ularning oldida hal qilinishi lozim bo‘lgan bir nechta muhim muammolarni hal qilish bo‘yicha ilmiy tadqiqotlar faol olib borilmoqda. Bu borada, perovskitning optoelektron xossalarini kuchaytirish, deffektlarni passivatsiya qilish va ularni kamaytirish yo‘llarini topish, qurilmalar barqarorligini oshirish muhim ilmiy ahamiyatga ega.

Respublikamizda ham so‘ngi yillarda alternativ quyosh elementlari bo‘yicha izchil fundamental va amaliy tadqiqotlarga alohida e‘tibor qaratilmoqda. Jumladan, perovskit quyosh element (PQE) larida konversiya ko‘rsatgichini yaxshilash, asosan foal qatlama maxsus qo‘shimchalar kiritish orqali optimal sharoyitlarini topish va ularning ro‘lini tushuninish va shular asosida olingan elementlarning barqarorligini o‘rganish bo‘yicha dastlabki qo‘yilgan qadamlarda salmoqli natijalarga erishilmoqda. Mazkur izlanishlar shuni ko‘rsatadiki, turli maxsus qo‘shimchalar yordamida perovskit foal qatlamining yakuniy donalarining o‘lchami kattalashishiga tasir qiladi va chegaraviy sirtlarining kamayishi evaziga, yuqori konversiya ko‘rsatkichiga ega fotovoltaik qurilmalarni olish imkonini beradi. Mamlakatimizni yanada rivojlantirish bo‘yicha Yangi O‘zbekistonning taraqqiyot strategiyasi¹ hamda 2030-yilgacha bo‘lgan ilm-fanni rivojlantirish konsepsiyasida² “ Qayta tiklanuvchi energiya manbalaridan foydalanishni kengaytirish va qo‘llab-quvvatlash..” vazifalari belgilangan. Ushbu yo‘nalishda qayta tiklanuvchi quyosh elementlarining yangi avlodini yaratish va ularni amaliyotga tatbiq etishga qaratilgan ilmiy-amaliy tadqiqotlar dolzarb ahamiyat kasb etadi.

Mazkur dissertatsiya ishi 2019-yil 21 maydagi O‘RQ-539-son “Qayta tiklanuvchi energiya manbalaridan foydalanish” to‘g‘risidagi O‘zbekiston respublikasining qonuni, 2019-yil 22-avgustdagi PQ – 4422-son “Iqtisodiy va ijtimoiy sohalarning energiya samaradorligini oshirish, energiya tejaydigan texnologiyalarni joriy etish va qayta tiklanadigan energiya manbalarini rivojlantirish bo‘yicha tezkor chora-tadbirlar to‘g‘risida” gi qarorlarda ko‘zda tutilgan ilmiy texnik vazifalarni hal qilishga qaratilgan. Qarorlaridagi hamda muqobil energetikadan foydalanishga oid boshqa me‘yoriy-huquqiy hujjatlarda belgilangan vazifalarni amalga oshirishda ushbu dissertatsiya tadqiqoti muayyan darajada xizmat qiladi.

¹ O‘zbekiston Respublikasi Prezidentining 2022-yil 28-yanvardagi PF-60-son «2022–2026-yillarga mo‘ljallangan Yangi O‘zbekistonning taraqqiyot strategiyasi to‘g‘risida» Farmoni;

² O‘zbekiston Respublikasi Prezidentining 2020-yil 29-oktabrdagi PF-6097-son «Ilm-fanni 2030-yilgacha rivojlantirish kontsepsiyasini tasdiqlash to‘g‘risida» Farmoni;

Tadqiqotning Respublika fan va texnologiyalarini rivojlanishi ustuvor yo‘nalishlariga mosligi. Ushbu dissertatsiya ishi O‘zbekiston Respublikasi fan va texnologiyalarni rivojlantirishning: III “Energetika, energoresurs tejamkorligi, transport, mashina va elektron asbobsozligi rivojlanishi”, II “Fizika, astronomiya, energetika va mashinasozlik” va VII. “Kimyoviy texnologiyalar va nanotexnologiyalar” kabi ustuvor yo‘nalishlariga muvofiq ravishda bajarilgan.

Muammoni o‘rganilganlik darajasi. Dunyoning ko‘plab yetakchi ilmiy markazlarida perovskit asosidagi quyosh elementlarida yuqori samaradorlikka erishish uchun ilmiy izlanishlar faol olib borilmoqda. Planar tuzilmali perovskit quyosh elementlari (PQE) bo‘yicha olib borilgan ilmiy yo‘nalishlarni rivojlantirishga Park N.G, Snaith H. J. va bir qator olimlar katta hissa qo‘shishgan. Dunyoning ko‘plab mamlakatlarida perovskitning kristall sifati, donachalar o‘shishi va barqarorlikni oshirishga qaratilgan ilmiy izlanishlar olib borilmoqda. Ushbu yo‘nalishda, additivlar yordamida kristallanish jarayonini boshqarish bo‘yicha Yang Yang, J. Hou va A. Hagfeldt guruhlari, morfologiyani optimallashtirish va yuqori sifatli qatlamlar olish yuzasidan A. Graetzel, M. Saliba hamda H. J. Snaith jamoalari va PQEning uzoq muddatli barqarorligini ta‘minlash maqsadida p–i–n tuzilmalarida interfeys muhandisligi bo‘yicha Y. L. Loo, S. R. Forrest va M. Graetzel guruhlari tomonidan olib borilgan ilmiy izlanishlarni alohida ta‘kidlab o‘tish zarur.

Respublikamizda mazkur yo‘nalish rivojiga akademik S.Sh. Rashidova, professorlar N. R. Ashurov jamoasi hamda B. L. Oksengendler, N. N. Turaeva, D. U. Matrasulov, E. Zaxidov, A. Zaxidov, va boshqalar o‘z ilmiy izlanishlari bilan organik–noorganik perovskitlar bo‘yicha o‘z hissalarini qo‘shgan.

Ushbu izlanishlarga qadar adabiyotlarda PQE samaradorligini belgilovchi asosiy omillardan biri bo‘lgan perovskit qatlamining morfologiyasini shakllantirish mexanizmlarini chuqur o‘rganish, xususan maxsus qo‘shimchalar kristall o‘shishiga ko‘rsatadigan ta‘sirning aniq mexanizmini ochib berish bo‘yicha yetarli ilmiy asoslar shakllanmagan. Bu esa aktiv qatlamning kristallanish jarayonini barqaror boshqarish va qurilma samaradorligini takrorlanuvchan holda ta‘minlash imkonini cheklaydi. Bundan tashqari, p–i–n tuzilishli PQElarda optimal morfologiya, optoelektron xususiyatlar va uzoq muddatli barqarorlikni turli tashqi omillar ostida baholash yuzasidan tizimli tadqiqotlar yetarli emas. Shu bois, yuqori samarali va barqaror PQE yaratish, hamda amaliy qo‘llanishda uchraydigan asosiy muammolarni bartaraf etish uchun mazkur yo‘nalishda chuqur fundamental va ilmiy-amaliy tadqiqotlar olib borish zaruratini yuzaga keltiradi.

Tadqiqotning dissertatsiya bajarilgan ilmiy-tadqiqot muassasasining ilmiy-tadqiqot ishi rejalari bilan bog‘liqligi. Dissertatsiya tadqiqoti O‘zbekiston Respublikasi Fanlar akademiyasi Polimerlar kimyosi va fizikasi instituti bazaviy ilmiy tadqiqot ishlari rejasi (2020–2024 y.) hamda REP-24112021/33 «Perovskite solar cells with optimized performance and stability» (2022–2024 y.) mavzularidagi fundamental loyiha doirasida bajarilgan.

Tadqiqotning maqsadi prekursor eritmalaridan perovskit absorber hosil bo'lishi kinetikasini ularning morfologiyasi bilan bog'liq holda o'rganish hamda maxsus qo'shimchani (tiomochevina) polikristallarning yiriklashuvdagi rolini va ularni invertlangan quyosh elementlarining samaradorligi va barqarorlik xususiyatlari bilan o'zaro bog'liqligini aniqlash.

Tadqiqotning vazifalari:

oralik komplekslar hosil bo'lishining turli erituvchilardagi prekursorlar konsentratsiyaga bog'liqligini o'rganish va perovskit absorberining morfologiyasini rivojlantirish uchun mas'ul bo'lgan strukturaviy parametrlarni aniqlash;

maxsus qo'shimcha tiomochevinaning – Lyuis asoslari sifatida perovskit absorber hosil bo'lishining barcha bosqichlarida (spinning, gaz-quenching va antisolvent qo'llash, termolish berish) tutgan rolini aniqlash;

spinning bosqichida qo'llaniladigan yondashuvlar – gaz quenching va antisolvent usullarini perovskit absorber morfologiyasini rivojlanish dinamikasi bo'yicha qiyosiy baholash;

optimal morfologik va optoelektron xususiyatlarga ega invertlangan quyosh elementlarini yaratish, ularning konversion ko'rsatkichlari bilan korrelyatsion bog'liqliklarini aniqlash;

p-i-n tuzilmasiga ega PQElarining barqarorligini turli sharoitlarda tekshirish.(interfeys muhandisligi (interface engineering) yordamida elementning barqarorligini oshirishdir)

Tadqiqot ob'yekti – MAPbI_3 , perovskit aktiv qatlamlari, PTAA- polimer yarim o'tkazgich kovak o'tkazuvchi qatlam sifatida. Maxsus qo'shimcha – tiomochevina (Thiourea) va SnOx elektron transport qatlamlari, ular asosidagi quyosh elementlari hisoblanadi.

Tadqiqotning predmeti prekursor siyohidagi kolloid qo'rg'oshin komplekslari, maxsus qo'shimcha qo'shilgan MAPbI_3 perovskitida donacha o'lchami, kristall tuzilishi, shuningdek ular asosidagi ITO/PTAA/ MAPbI_3 /PCBM/AZO/(SnOx)/Ag tuzilmasiga ega quyosh elementlari, optik, optoelektron, fotovoltaiik va barqarorlik xususiyatlarini tadqiq qilishdan iborat.

Tadqiqotning usullari. PQElarini tayyorlashda spin-koating, antierituvchi, gaz bilan sovutish , maxsus qo'shimchalar, termik ishlov berish usullaridan foydalanildi. XRD, GIWAXS, SEM, UPS, AFM, YaMR spektroskopiyasi tadqiqotlar usullaridan perovskitlardagi kristall panjara va morfologiyani o'rganish uchun foydalanildi. UV-Vis hamda in situ UV-Vis absorbsion optik spektroskopiyasi, stasionar va kechikkan fluoressensiya, Raman spektroskopiyasi, ultrabinafsha fotoelektron spektroskopiyasi va rentgen nurlari fotoelektron spektroskopiyasi usullari orqali na'munalarning optik va elektron parametrlari tadqiq qilindi. Volt – amper xarakteristikasi, elektrokimyoviy impedans spektroskopiyasi, usullaridan qurilmalarning samaradorligi, kabi parametrlarni aniqlashda foydalanildi. Barqarorlik sinovlari maksimal chiqish quvvati, usullari va boshqa standart protokollar yordamida bajarilgan.

Tadqiqotning ilmiy yangiligi quyidagilardan iborat:

ilk bor perovskit absorber shakllanishida erituvchi turidan qat'iy nazar, prekursor konsentratsiyasi ortishi bilan poliyodid komplekslarining o'sish qonuniyati aniqlangan;

ilk bor tiomochevina qo'shimchasining perovskit kristallanish jarayonidagi roli aniqlangan;

ikki qatlamli AZO/SnO_x elektron ekstraksiya qatlami (EEL) asosida barqaror MAPbI₃ga asoslangan p-i-n strukturaga ega quyosh elementi ishlab chiqildi, bunda SnO_x qatlami ion migratsiyasi va elektrod korroziyasini samarali bostiruvchi ko'p funksional to'siq sifatida ishlashi aniqlangan;

Tadqiqotning amaliy natijalari quyidagilardan iborat:

poliyodid perovskitga o'xshash strukturalarning yagona o'sish qonuniyati aniqlanib, erituvchi turidan mustaqil ekani va konsentratsiya ortishi bilan yuzaga chiqishi ko'rsatildi. Ushbu xulosa ²⁰⁷Pb YaMR, UV-Vis, UPS va elektr o'tkazuvchanlik o'lchovlari orqali miqdoriy tasdiqlandi;

ilk bor tiomochevina qo'shimchasi mavjudligida perovskit absorberning struktural evolyutsiyasi to'liq tushuntirib berildi.

YaMR va UPS natijalari ushbu effektning ionlarning yuqori harakatchanligi bilan bog'liq ekanini ko'rsatdi, bu ehtimol tiomochevina molekularining termal sharoitlarda yuqori harakatchanligidan kelib chiqadi. Umumiy holda, bu natijalar tiomochevinaning kristall o'sishini osonlashtiruvchi mexanizmini izchil tushuntirib berdi;

yuqori vakuum sharoitida issiqlik stressi sinovi PQElarida interfeys muhandisligining muhim rolini tasdiqladi. SnO_x qatlamining kiritilishi Ag elektrod korroziyasini samarali ravishda bostirdi va fizik hamda elektr mustahkamlikni yaxshiladi.

Tadqiqot natijalarining ishonchliligi. Dissertatsiya ishida perovskit quyosh elementining barcha parametrlarini aniqlash uchun zamonaviy tadqiqot usullaridan foydalanilgan. Strukturaviy, optik, elektron, fotovoltaik va barqarorlik tadqiqotlarining natijalari bir-birini tasdiqlaydi. Tasodifiy tabiatga ega miqdorlarni tahlil qilish uchun har bir turdagi qurilmadan 10 tadan tayyorlangan va ularning parametrlari bir hil sharoitlarda o'lchandi. Olingan ilmiy va amaliy natijalar qator respublika va xalqaro ilmiy anjumanlarda muhokama qilingan.

Tadqiqot natijalarining ilmiy va amaliy ahamiyati. Tadqiqot natijalarining ilmiy ahamiyati shundan iboratki, perovskit absorber shakllanish jarayonida poliyodid komplekslarining konsentratsiyaga bog'liq o'sish qonuniyati universal ekanligi va erituvchi turidan mustaqilligi eksperimental usullar (²⁰⁷Pb YaMR, UV-Vis, UPS, o'tkazuvchanlik o'lchovlari) orqali miqdoriy tasdiqlandi. Tiomochevina qo'shimchasining perovskit kristallanish dinamikasidagi roli aniqlandi; uning termik ishlov davrida faollashib, kristallarning <110> yo'nalishi bo'yicha qayta yo'nalishi va o'sishini rag'batlantirishi, bu effektning ionlarning yuqori harakatchanligi bilan bog'liqligi isbotlandi.

Tadqiqot natijalarining amaliy ahamiyati shundan iboratki, ikki qatlamli AZO/SnO_x elektron ekstraksiya qatlami asosida ishlab chiqilgan ITO/PTAA/MAPbI₃/PCBM/AZO/(SnO_x)/Ag tuzilmasiga ega barqarorroq va yuqori samarali PQElarini yuqori vakuum sharoitida issiqlik stressiga chidamli bo‘lib, SnO_x qatlami namlik va parchalanish mahsulotlarining kirishini oldini olgan holda, elektrod korroziyasini samarali bostirdi va qurilmaning ishlash muddatini uzaytirish ikmoniyatlari mavjudligi tadqiq qilindi.

Tadqiqot natijalarining joriy qilinishi. “Perovskit yutuvchi qatlamining shakllanish xususiyatlari bilan unga asoslangan quyosh elementlarining konversiya ko‘rsatkichlari o‘rtasidagi bog‘liqlik” mavzusi bo‘yicha olingan ilmiy natijalar asosida:

tiomochevina kabi maxsus qo‘shimchalar (additive) aktiv qatlamga kiritish orqali va aktiv qatlam ustida o‘stirilgan SnO_x qatlamli zich to‘siq ko‘rsatilgan FA S.A.Azimov nomidagi Fizika-texnika institutida bajarilayotgan IL-5421101892 raqamli “Yarim o‘tkazgichli perovskitlarga asoslangan energiya tejamkor tuzilmalarning yorituvchanlik xususiyatlarining fundamental asoslarini o‘rganish” mavzusidagi fundamental loyihasini bajarishda foydalanilgan (2025-yil 8-sentyabr №01/467 raqamli ma’lumotnoma). Muvaffaqiyatli qo‘llanilgan tiomochevina(SC(NH₂)₂) kabi maxsus qo‘shimchalar (additive) kiritish orqali CsPbBr₃ aktiv qatlamidagi kristallitlar (grain) o‘lchami kattalashtirilishi aniqlangan. SnO_x elektron ekstraksiya qatlami (EEL) arxitekturasida CsPbBr₃ asosidagi fotosezgir qurilmalarda qurilmalarning uzoq muddatli ishlash barqarorligiga erishilgan.

NATOning “Tinchlik va xavfsizlik yo‘lida fan” (SPS) dasturi tomonidan moliyalashtirilgan, Vuppertal “Aqlli materiallar va tizimlar” markazi (Wuppertal, Germaniya) va Polimerlar kimyosi va fizikasi instituti (Toshkent, O‘zbekiston) hamkorligidagi “Light Harvesting in Space with Perovskite Solar Cells (SpacePerCells)” mavzusidagi xalqaro loyihada foydalanilgan. Dissertatsiyada ishlab chiqilgan va ITO/PTAA/MAPbI₃/PCBM/EEL/Ag qurilma arxitekturasida qo‘llanilgan AZO/SnO_x ikki qatlamli elektron ekstraksiya qatlami (EEQ) quyosh elementlarining uzoq muddatli ishlash barqarorligi va chidamliligini sezilarli darajada oshirish imkonini bergan. Xususan, ushbu elektron ekstraksiya qatlami samarali o‘tkazmaydigan to‘siq (permeation barrier) vazifasini bajarib, perovskit qatlamidagi mobil ionlar migratsiyasini to‘shish hamda galoid birikmalarining tashqariga chiqib ketishini oldini olishda muvaffaqiyatli qo‘llanilgan. Bu natijalar kosmik sharoitlar uchun xos bo‘lgan past bosim (vakuum) sharoitida qurilmalarning funksional ko‘rsatkichlarini saqlab qolish imkonini bergan. (Tasdiqlovchi hujjat: Vuppertal universiteti professorining tavsiyanomasi va hamkorlik loyihasi ma’lumotnomasi).

Tadqiqot natijalarining aprobatsiyasi. Dissertatsiya bo‘yicha olingan asosiy natijalar 2 ta xalqaro va 4 ta respublika ilmiy-amaliy anjumanlarida ma’ruza qilingan va muhokamadan o‘tkazilgan.

Tadqiqot natijalarining e‘lon qilinishi. Dissertatsiya mavzusi bo‘yicha jami 10 ta ilmiy ish chop etilgan, bulardan O‘zbekiston Respublikasi Oliy Attestatsiya komissiyasining falsafa doktori (PhD) dissertatsiyalari asosiy ilmiy nashrlarini chop

etishga tavsiya etilgan ilmiy nashrlarda 5 ta ilmiy maqola, jumladan, 3 ta respublika va 2 ta xorijiy jurnallarda nashr etilgan.

Dissertatsiyaning tuzilishi va hajmi. Dissertatsiya tarkibi kirish qismi, olti bob, xulosa, foydalanilgan adabiyotlar ro'yxati va ilovalardan iborat. Dissertatsiyaning hajmi 102 betni tashkil etadi.

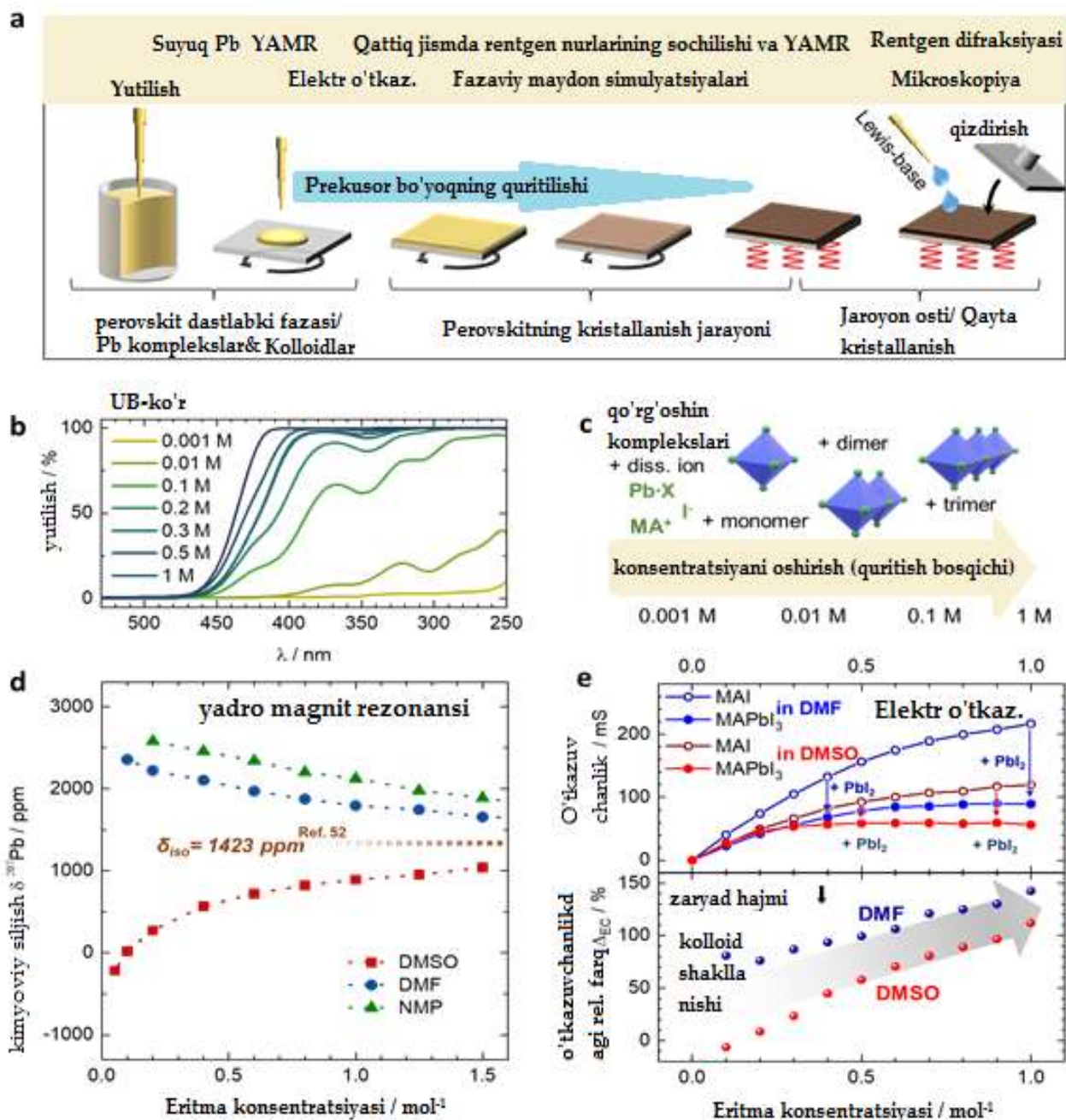
DISSERTATSIYANING ASOSIY MAZMUNI

Kirish qismida dissertatsiya mavzusining dolzarbligi va zarurati asoslangan, tadqiqotning maqsad va vazifalari, obyektlari va predmetlari belgilangan, O'zbekiston Respublikasida fan va texnologiyalarni rivojlantirishning ustuvor yo'nalishlariga mosligi ko'rsatilgan, uning ilmiy yangiligi va amaliy natijalari bayon qilingan, olingan natijalarning ishonchliligi asoslangan, nazariy va amaliy ahamiyati ochib berilgan, tadqiqot natijalarining amaliyotga joriy etish istiqbollari bo'yicha xulosa qilingan hamda nashr etilgan ilmiy ishlar va dissertatsiya tuzilishi bo'yicha ma'lumotlar keltirilgan.

Dissertatsiyaning **“Yuqori sifatli perovskit plyonkalarini olish muammosining hozirgi holati, quyosh elementlarini yaratish va barqarorlashtirish strategiyalari”** nomli **birinchi bobida** perovskit yupqa qatlamlarining hosil bo'lishi, xususan, eritmadan qayta ishlash jarayonidagi murakkabliklar, kristallarning yadrolanishi va o'sish mexanizmlari, shuningdek, prekursor eritmasining holati va uning ta'siri batafsil yoritilgan. Shu bilan birga, spin-coating va termik annealing kabi asosiy texnologik jarayonlarning perovskit plyonkalari sifatiga ta'siri, ularning nazariy asoslari va qo'shimchalarning kristall donachalari o'lchami, yo'nalishi va nuqsonlarga ta'sirini o'rganishga bag'ishlangan adabiyotlar sharhi keltirilgan. Ushbu bobda perovskit qurilmalarining barqaror va takrorlanadigan natijalariga erishish uchun eritma kimyosi, qoplama jarayoni va qattiq fazaga o'tish o'rtasidagi bog'liqlikni chuqurroq o'rganish zarurligi ta'kidlangan.

Dissertatsiyaning **"Tadqiqot obyektlari va usullari"** deb nomlangan **ikkinchi bobida** PQE larini tayyorlash va tavsiflash uchun foydalanilgan usullar va texnologiyalar batafsil bayon etilgan. Bobda qurilmaning tuzilishi, har bir qatlamning (SnO₂, perovskit aktiv qatlami va kumush ustki elektrod) funksiyalari va ularni tayyorlashning o'ziga xos jarayonlari tushuntirilgan. Shuningdek, tadqiqotda qo'llanilgan optik, kristallografik, morfologik, reologik va elektrofizik xususiyatlarni aniqlashga qaratilgan asboblari va usullari (jumladan, UV-Vis, XRD, AFM, FTIR, SEM,) haqida ma'lumotlar keltirilgan. Qurilmalarning samaradorligi va fotovoltaiq parametrlari quyosh simulyatori yordamida I-V va IS o'lchovlari orqali baholangani ham yoritilgan.

Dissertatsiyaning **“Invertirlangan PQE larida tiomochevina qo'shimchasi yordamida Lyuis asos-vositasida kristallanishni boshqarish”** deb nomlangan **uchinchi bobida** perovskit aktiv qatlamini shakllantirish jarayonlari chuqur o'rganilgan. Bobning asosiy maqsadi prekursor eritmalarni spin-coating va termik annealing usullari bilan tayyorlashda maxsus qo'shimchalarning, xususan,

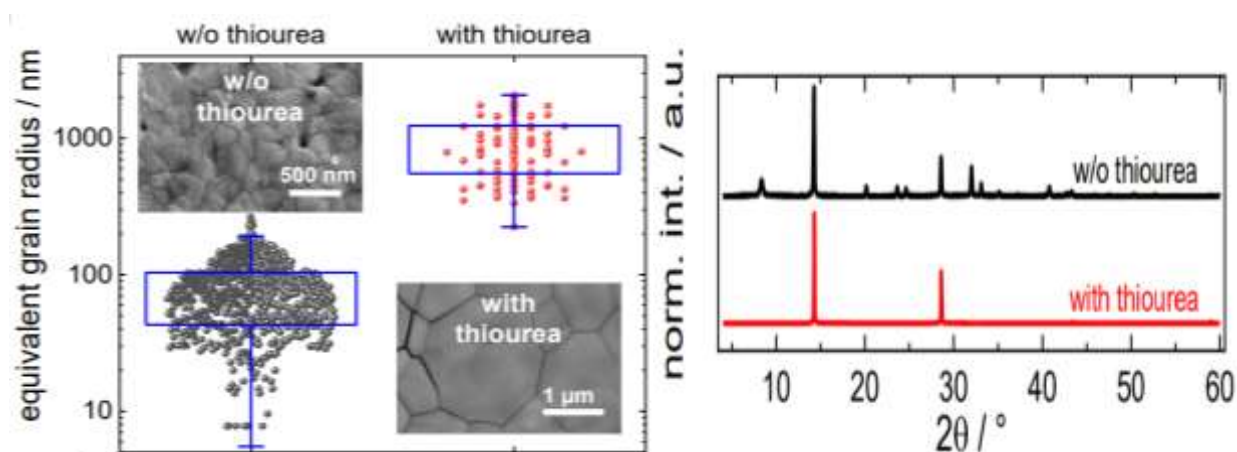


1-rasm: Erituvchi kimyosi (turi va konsentratsiyasi): a) Perovskitni cho'ktirish va o'lchash usullarining sxematik ko'rinishi. b) DMF eritmasida turli konsentratsiyalarda MAPbI₃ siyohlarining UB-ko'r. yutilishi . c) Konsentratsiyaga bog'liq holda qo'rg'oshin kompleksining evolyutsiyasi tasviri. d) DMF, DMSO va NMP eritmalarida MAPbI₃ siyohlarining ²⁰⁷Pb YAMR spektri, prekursor molyar konsentratsiyasiga nisbatan; nuqtali chiziq qattiq holatdagi MAPbI₃ ni belgilaydi. e) MAPbI₃ va MAI ning DMF, DMSO va NMP eritmalaridagi turli konsentratsiyalardagi elektr o'tkazuvchanligini taqqoslash; pastki panelda esa nisbiy elektr o'tkazuvchanlik farqi (ΔEC) ko'rsatilgan.

tiomochevinaning (NH₂-CS-NH₂) perovskit kristallanishi, morfologiyasi va optoelektronik xususiyatlariga ta'sirini aniqlashdan iborat. Bobda, avvalambor perovskit yupqa qatlamlarining hosil bo'lish mexanizmi tahlil qilingan. Bu jarayon bir necha bosqichdan iborat bo'lib, u LaMer yadrolanish nazariyasi va Lewis kislotasi/asos o'zaro ta'siri modeli asosida tushuntirilgan. Ushbu modelga ko'ra,

erituvchi molekulari (asos sifatida) qo‘rg‘oshin komponentlari (kislota sifatida) bilan oraliq komplekslar hosil qiladi. Bu komplekslar perovskitning kristallanishini kechiktirib, yupqa qatlamning sifatini nazorat qilish imkonini beradi. Tadqiqotda turli xil donor xususiyatiga ega erituvchilar – DMF, DMSO va NMP tanlangan. Eritmalar konsentratsiyasining o‘zgarishi bilan hosil bo‘ladigan polikomplekslarning xususiyatlari UV-Vis spektroskopiyasi, ^{207}Pb NMR spektroskopiyasi va o‘tkazuvchanlik o‘lchovlari yordamida o‘rganilgan (**1-rasm**). Olingan natijalar, eritma konsentratsiyasi oshishi bilan poliyodid komplekslarining hajmi o‘sib borishini ko‘rsatdi, bu esa zaryad-hajm nisbatining kamayishiga olib keladi.

Tadqiqotning muhim qismi sifatida, perovskit eritmasiga tiomochevina qo‘shimchasi kiritilib, uning ta‘siri o‘rganildi. Tiomochevina neytral molekula bo‘lganligi sababli, u eritmada ion muvozanatini buzmaydi va bu uni samarali qo‘shimcha sifatida ishlashiga yordam beradi. Tajribaviy natijalar shuni ko‘rsatadiki, tiomochevina mavjud bo‘lganda perovskit donachalari hajmi sezilarli darajada oshadi, bu esa qurilmalarda nuqsonlarning kamayishiga va barqarorlikning yaxshilanishiga olib keladi (**2-rasm**). Rentgen difraksiyasi (XRD) va scanning electron microscopy (SEM) tahlillari qo‘shimcha kiritilgan namunalarda kristall donachalarining o‘lchami kattalashganligini tasdiqladi.

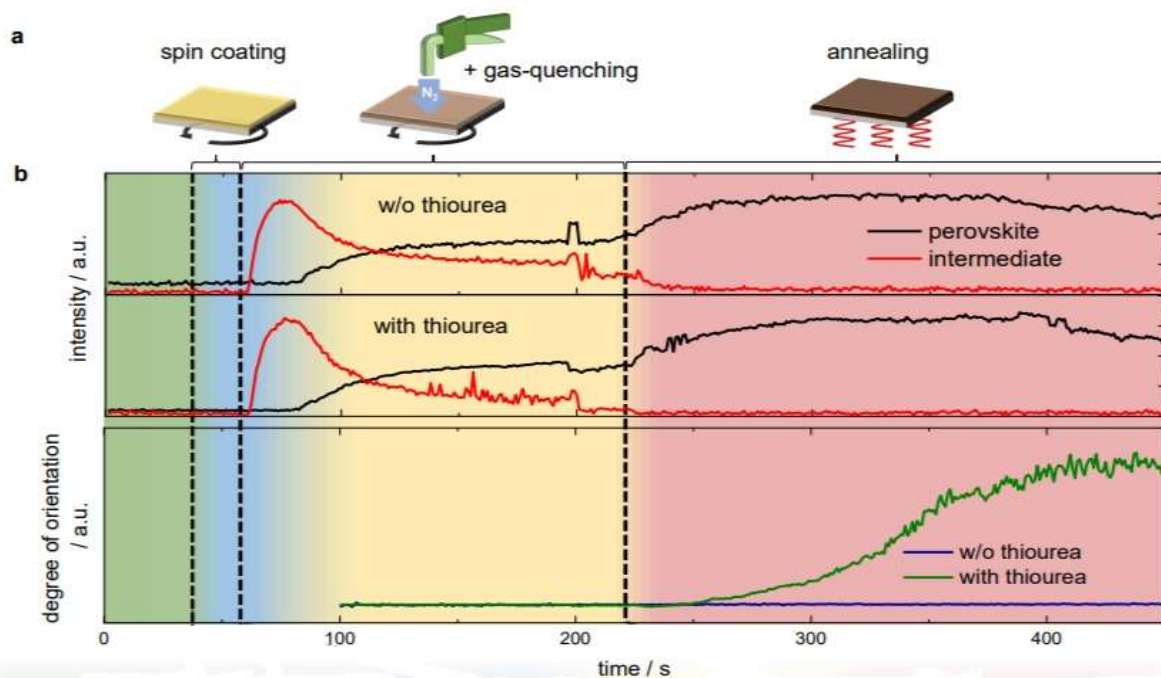


2-rasm: Tiomochevina(thiourea) qo‘shimchasining ta‘siri. a) DMF:NMP prekursor siyohidan gaz bilan sovitish (gas quenching) orqali 1.0 M konsentratsiyada, 0.1 M tiomochevina(thiourea) qo‘shimchasi bilan(with) va usiz(w/o) tayyorlangan MAPbI₃ qatlamlarining donacha o‘lcham taqsimoti va SEM tasvirlari. b) 0.1 M tiomochevina(thiourea) qo‘shimchasi bilan(with) va usiz(w/o) tayyorlangan qatlamlarning rentgen difraksiyasi spektrlari.

Perovskit strukturasi evolyutsiyasini real vaqt rejimida kuzatish uchun in situ GIWAXS (Grazing-Incidence Wide-Angle X-ray Scattering) kabi zamonaviy sinxrotron texnikalari qo‘llanilgan (**3-rasm**).

Tadqiqot natijalari shuni ko‘rsatdiki, tiomochevina qo‘shimchasi mavjud bo‘lgan namunalarda termik annealing bosqichida kristallitlar sezilarli darajada qayta yo‘nalgan va yuqori darajada tartiblangan perovskit domenlari hosil bo‘lgan. (Pastki qism) 90°/45° intensivlik nisbati orqali aniqlangan yo‘nalishli tartib donachalar o‘sishida ustun yo‘nalish mavjudligini bildiradi, bu tiomochevina bilan yanada kuchayadi. Barcha namunalarda 7:3 nisbatdagi DMF:NMP erituvchi aralashmasida

tayyorlangan. 200 soniya atrofida kuzatilgan artefaktlar spin-coating jarayonining tugashiga to‘g‘ri keladi.



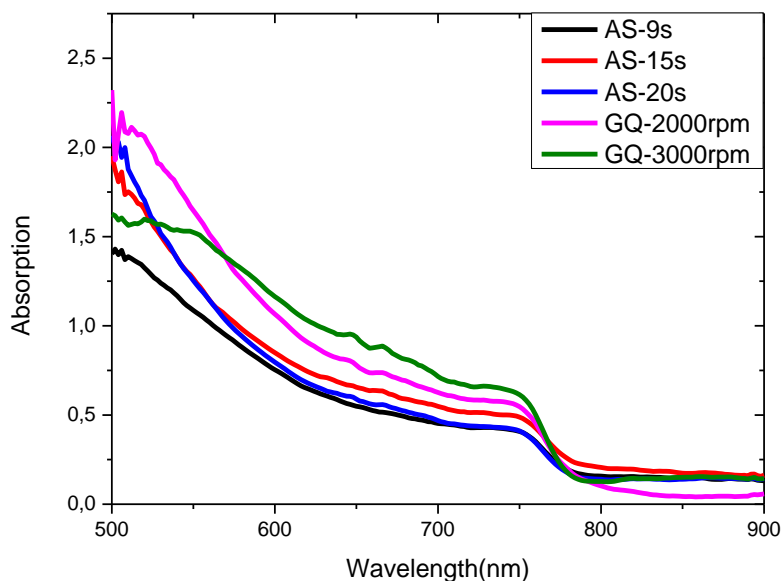
3-rasm: Perovskit hosil bo‘lish jarayoni. a) In situ cho‘ktirish tajribasining sxematik ko‘rinishi. b) Vaqtga bog‘liq holda perovskit va $PbI_2 \cdot NMP$ oraliq fazasining GIWAXS intensivliklari (tимоchevina(thiourea) bilan(with) va usiz(w/o)), ularning nisbiy faza tarkibini ko‘rsatadi.

Xulosa qilib aytganda, bobda olingan eksperimental va nazariy natijalar timochevinaning perovskit plyonkasi hosil bo‘lishida muhim rol o‘ynashini ko‘rsatdi. Uning qo‘rg‘oshin va yodid ionlari bilan dinamik o‘zaro ta’siri orqali ionlarning harakatchanligi oshadi, bu esa donachalarning yanada samarali o‘shishiga va yuqori sifatli, kam nuqsonli perovskit filmlari hosil bo‘lishiga olib keladi.

Dissertatsiyaning "**Perovskit quyosh elementlarida aktiv qatlamning kristallanishini nazorat qilish uchun anti-solvent va gaz bilan sovitish usullari**" deb nomlangan **to‘rtinchi bobida** perovskit plyonkalarini tayyorlashda eng muhim qiyinchiliklardan biri bo‘lgan kristallanish jarayonini aniq nazorat qilish muammosi tahlil qilingan. Bobda yuqori sifatli va uzoq muddat barqaror perovskit qatlamini shakllantirish uchun keng qo‘llaniladigan anti-solvent va gaz bilan sovitish usullari o‘rganilgan.

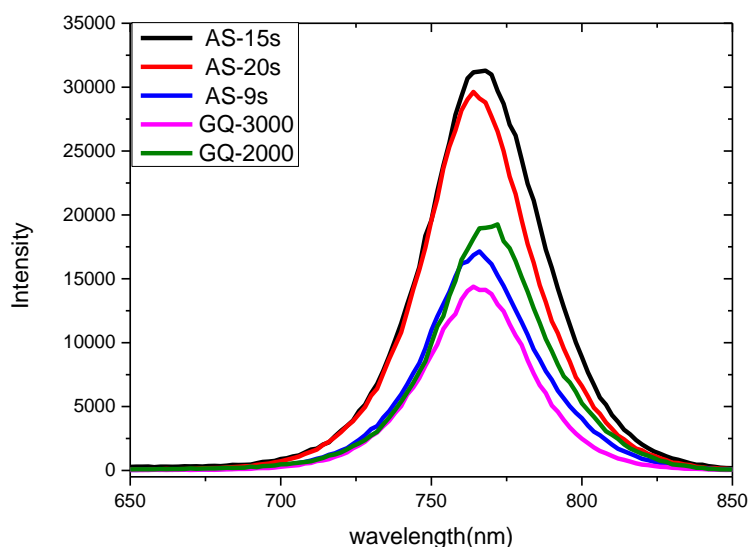
Tadqiqotda gaz bilan sovitish usuli ancha istiqbolli alternativa sifatida keltirilgan. Bu usul, inert gaz (azot) yordamida erituvchini tezkor bug‘latib yuborish orqali kristallanishni nazorat qiladi. Uning asosiy afzalliklari sifatida jarayonni nozik sozlash (gaz oqimi tezligi, sovitish davomiyligi), bir xil, tekis yuzali va nuqsonlar kam bo‘lgan plyonkalar hosil qilish hamda keng miqyosda ishlab chiqarish imkoniyatlari ko‘rsatilgan. Bobning asosiy qismi anti-solvent va gaz bilan sovitish texnikalarining optik va strukturaviy xususiyatlariga ta’sirini taqqoslab o‘rganishga bag‘ishlangan.

Bundan tashqari, UV-Vis spektroskopiyasi orqali gaz bilan sovitish usulida olingan plyonkalar butun UV-ko‘rinuvchi spektrda yorug‘likni ancha samaraliroq yutishi aniqlandi (**4-rasm**).



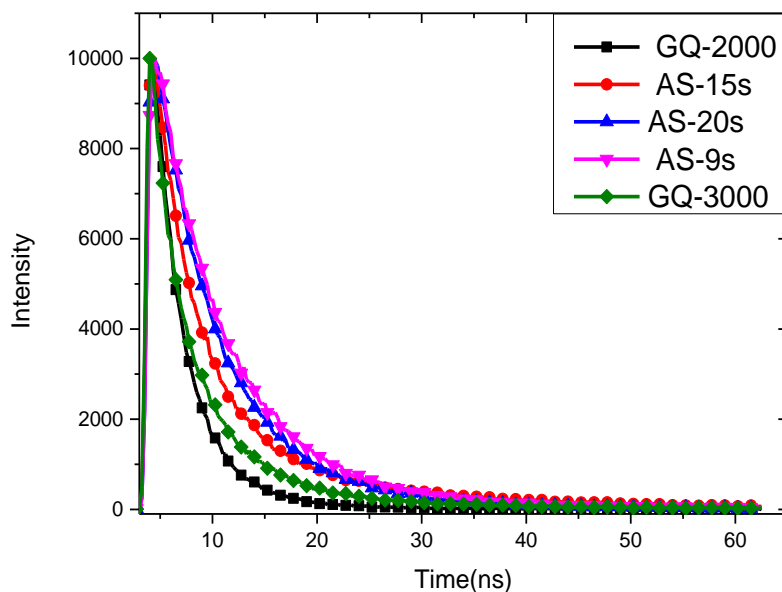
4-rasm: ITO shisha/PTAA/perovskitning yutilishi (Absorption).
Gaz bilan sovitish (GQ) va anti-erituvchi (AS) usullarining taqqoslanishi.

Ayniqsa, 550 nm to‘lqin uzunligida yutilish koeffitsienti 1.5 dan oshgani, bu aktiv qatlamlarning yorug‘likni yutish (light-harvesting) qobiliyati yuqori ekanligini isbotlaydi. PL (Photoluminescence) va TRPL (Time-Resolved Photoluminescence) o‘lchovlari ham gaz bilan sovitish usulining ustunligini ko‘rsatdi. Gaz bilan sovitilgan namunalarda PL intensivligi ancha past bo‘lgan, bu esa zaryadni ajratib olish jarayoni yanada samaraliroq ekanligini yoki non-radiativ rekombinatsiya yo‘qotishlarining kamayganligini anglatadi (5-rasm).



5-rasm: ITO shisha/PTAA/MAPbI₃ ning barqaror holatdagi fotolyuminessensiyasi (PL). Gaz bilan sovitish (GQ) va anti-erituvchi (AS) usullarining taqqoslanishi.

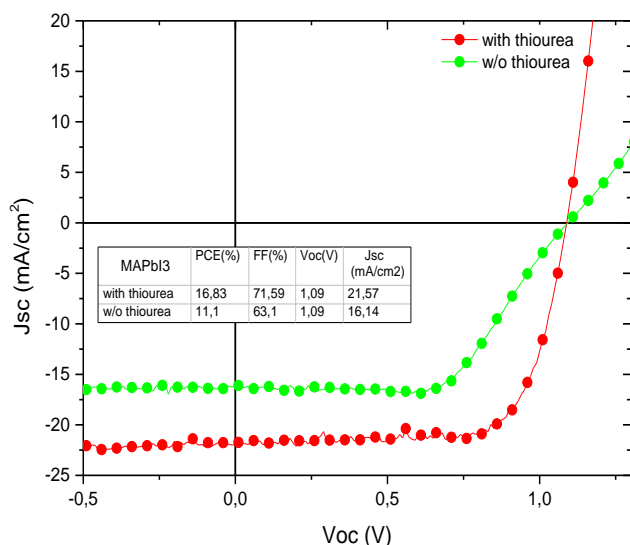
TRPL tahlillari esa gaz bilan sovitish usuli yordamida olingan namunalarda tez (τ_1) va sekin (τ_2) parchalanish komponentlarining qiymatlari optimallashtirilganini ko‘rsatdi (6-rasm). Bu holat perovskit qatlamidagi nuqsonlar zichligining pasayganligi va yig‘ish jarayonining yaxshilanganligidan dalolat beradi.



6-rasm. ITO shisha/PTAA/perovskit ning vaqtga bog‘liq fotolyuminessensiya (TRPL) spektrlari. Gaz bilan sovitish (GQ) va anti-erituvchi (AS) usullarining taqqoslanishi.

Xulosa qilib aytganda, tadqiqot natijalari gaz bilan sovitish usuli perovskit fazasining morfologiyasini shakllantirishda ancha istiqbolli ekanligini ko‘rsatadi. Ushbu usul bir necha yuz nanometrgacha bo‘lgan polikristallarning o‘shishiga yordam beradi. Bunday morfologiyaning rivojlanishi perovskitning optoelektronik xususiyatlarini yaxshilaydi, taklif qilingan yondashuv esa qurilmalarning sanoat namunalarini ishlab chiqarish uchun juda mos keladi.

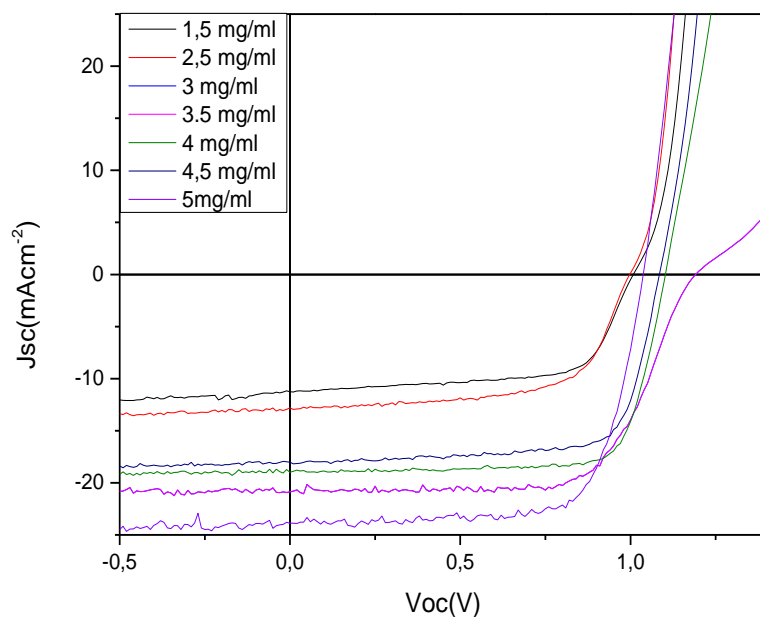
Dissertatsiyaning "**Tiomochevina qo‘shimchasi va gazni sovitish usuli bilan perovskit asosidagi quyosh elementi yaratish**" nomli **beshinch**i bobida yuqori samaradorlikka ega bo‘lgan teskari (p-i-n) PQElarini ishlab chiqarish va ularning ishlash mexanizmlari batafsil o‘rganilgan. Bobda, avvalgi tadqiqotlar natijalariga tayanib, tiomochevina qo‘shimchasi va gazni sovitish texnologiyalarini birgalikda qo‘llash orqali qurilma samaradorligini sezilarli darajada oshirishga e‘tibor qaratilgan.



7-rasm. Tiomochevina(thiourea) qo‘shimchasi bilan(with) va usiz(w/o) tayyorlangan invers perovskit quyosh elementining J–V xarakteristikasi.

Tadqiqot natijalariga ko'ra, tiomochevina qo'shilgan namunalarda 16.83% gacha yuqori quvvat konversiyasi samaradorligi (PCE) kuzatilgan, nazorat (qo'shimchasiz) namunalari esa bor-yo'g'i 11.1% samaradorlikni namoyish etgan (7-rasm). Bu topilmalar, tiomochevinaning Lewis asosi sifatida perovskitning fotovoltaik ishlashini va aktiv qatlam sifatini yaxshilashdagi muhim rolini isbotlaydi. Xulosa qilib aytganda, bobda tiomochevina qo'shimchasi va gazni sovitish usulidan foydalanib, p-i-n tuzilishiga ega quyosh elementlari yaratilgan. Ushbu qurilmalar 12% dan 16% gacha takrorlanuvchan yuqori quvvat konversiya samaradorligini namoyish etgan.

Bobning ikkinchi bo'limida p-i-n turdagi perovskitli quyosh elementlarida kovak o'takuvchi qatlam sifatida ishlatiladigan PTAA eritmasining optimal konsentratsiyasi aniqlandi. Qurilmalarning J-V xarakteristikalari turli konsentratsiyalardagi (1,5-5 mg/ml) qiymatlari o'lchandi va taqqoslandi. Natijalar shuni ko'rsatdiki, PTAA ning past konsentratsiyalarida Jsc, Voc, PCE va FF kabi asosiy parametrlar past qiymatlarga ega bo'ldi. Bu ingichka yoki to'liq bo'lmagan HTL bilan bog'liq bo'lib, qurilmaning ketma-ket qarshiligini oshirdi. Aksincha, konsentratsiya oshirilganda (3-5 mg/ml), to'ldirish koeffitsiyenti (FF) sezilarli darajada yaxshilandi, bu esa HTL va perovskit qatlami o'rtasidagi aloqa



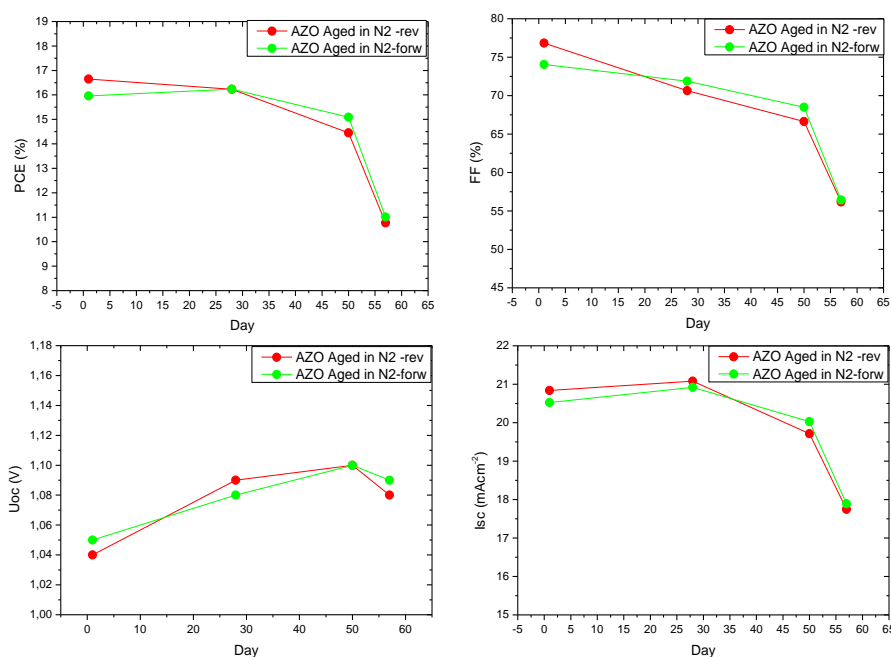
8-rasm: Turli konsentratsiyadagi PTAA/Toluol (1,5 – 5 mg/ml) bilan tayyorlangan perovskit quyosh elementining J–V xarakteristikalari.

yaxshilanganligini ko'rsatadi. Eng yuqori samaradorlik 5 mg/ml konsentratsiyada kuzatildi, bu yerda PCE 17,3% ga yetdi, Voc 1,05 V va Jsc 22 mAcm⁻² (8-rasm).

Dissertatsiyaning "**Invertirlangan PQElarida ikki qatlamli AZO/SnO_x elektron ekstraksiya interfeysi orqali barqarorlikni oshirish yo'llari**" deb nomlangan **oltinchi bobida** PQElarining tijoratlashuviga to'sqinlik qiluvchi eng muhim muammolardan biri operatsion barqarorlik masalasi chuqur o'rganilgan.

Bobning asosiy maqsadi SnO_x qo‘shimcha qatlamining MAPbI_3 asosidagi qurilmalarning termik, fotostrukturaviy va operatsion barqarorligini oshirishdagi rolini tizimli tahlil qilishdan iborat. Bu o‘rganish yuqori vakuum va uzluksiz yorug‘lik sharoitida o‘tkazilgan keng qamrovli sinovlarga asoslanadi. Tadqiqotda ITO/PTAA/ MAPbI_3 /PCBM/AZO/ (SnO_x) /Ag arxitekturasiga ega bo‘lgan qurilmalar yaratilib, ularning yuqori vakuum (10^{-4} mbar) va uzluksiz yorug‘lik (520 nm LED, 20 mW/cm^2) sharoitida ishlash barqarorligi sinovdan o‘tkazilgan.

Bobning alohida bo‘limida turli sharoitlarda yuzaga keladigan degradatsiya mexanizmlari yoritilgan. Namlik va kislorodning perovskit materialiga ta‘siri tahlil qilingan. Suv bug‘lari ishtirokida perovskitning $\text{CH}_3\text{NH}_3\text{PbI}_3 \rightarrow \text{CH}_3\text{NH}_3\text{I} + \text{PbI}_2$ kabi reaksiyalar orqali parchalanishi sodir bo‘lishi va bu parchalanishning qayta tiklanmasligiga sabab bo‘lishi aytilgan. N_2 atmosferasida yuzaga keladigan degradatsiya mexanizmi esa kamroq shikast yetkazadi, asosan ion migratsiyasi bilan bog‘liq bo‘ladi va qisman qayta tiklanishi mumkinligi ko‘rsatilgan (**9-rasm**).

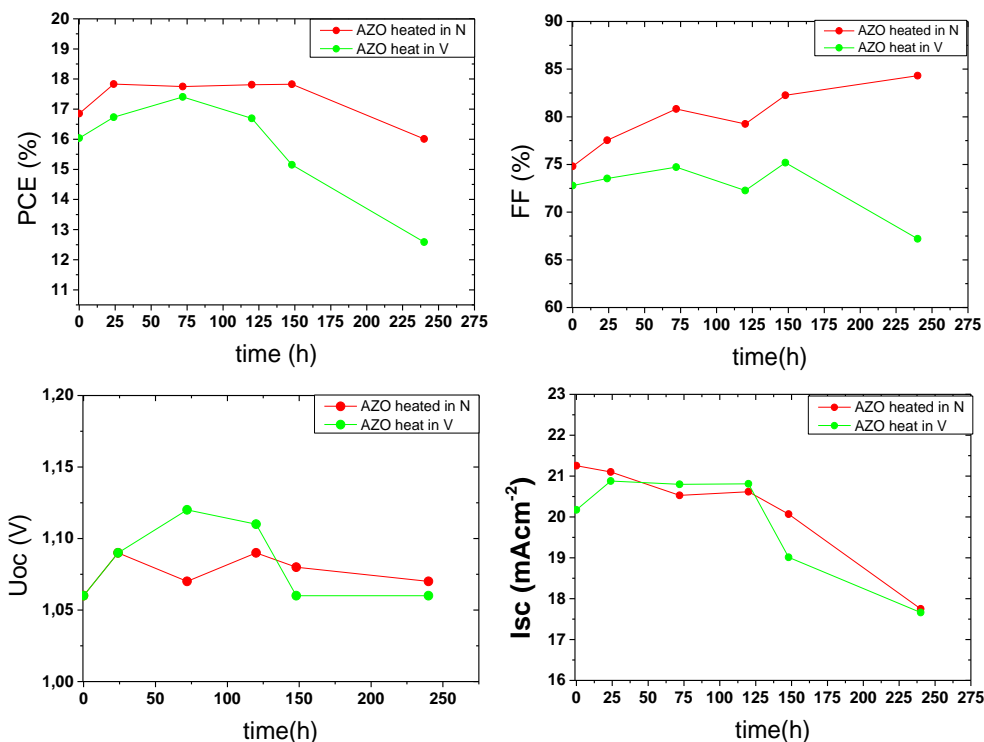


9-rasm: Azot(N_2) muhitida qaritilgan (aged) quyosh elementining barqarorligi.

Yuqori harorat ostidagi barqarorlik sinovlari ham katta ahamiyatga ega bo‘lgan. 60°C haroratda o‘tkazilgan testlar shuni ko‘rsatdiki, vakuum sharoitida saqlangan namunalar N_2 atmosferasidagi namunalarga nisbatan tezroq degradatsiyaga uchragan (**10-rasm**). Vakuum sharoitida PCE 16% dan 12% gacha pasaygan, holbuki, N_2 muhitida atigi 0.5% ga kamaygan. Bu natijalar vakuumning ion migratsiyasini kuchaytirishi va aktiv qatlamning parchalanishiga sabab bo‘lishini tasdiqlaydi. Tadqiqotda shuningdek, yuqori harorat ostida Ag elektrodlarida yuzaga kelgan korroziya (qorayish) vizual ravishda hujjatlashtirilgan, bu esa SnO_x qatlamining ushbu jarayonni samarali to‘xtatishini ko‘rsatgan. Shu bilan birga, J–V xarakteristikalarining kengaytirilgan tahlilida SnO_x qatlamining himoyalovchi bufer vazifasini bajarishi, namlik kirishini, ion migratsiyasini va interfeys yomonlashuvini

samarali bostirishi qayd etilgan. **11-rasmda** MAPbI₃ asosidagi PQElarining yuqori vakuum (10⁻⁴ mbar) sharoitida barqarorligi. MAPbI₃ asosida ishlab chiqilgan

ITO/PTAA/MAPbI₃/PCBM/AZO/(SnO_x)/Ag tuzilmasiga ega quyosh elementlarining ishlash barqarorligi 4 kun davomida uzluksiz yoritish (LED, 520 nm, 20 mW/sm²) ostida tekshirildi. Taqqoslash uchun SnO_x qatlami bilan va usiz qurilmalar o'rganildi.

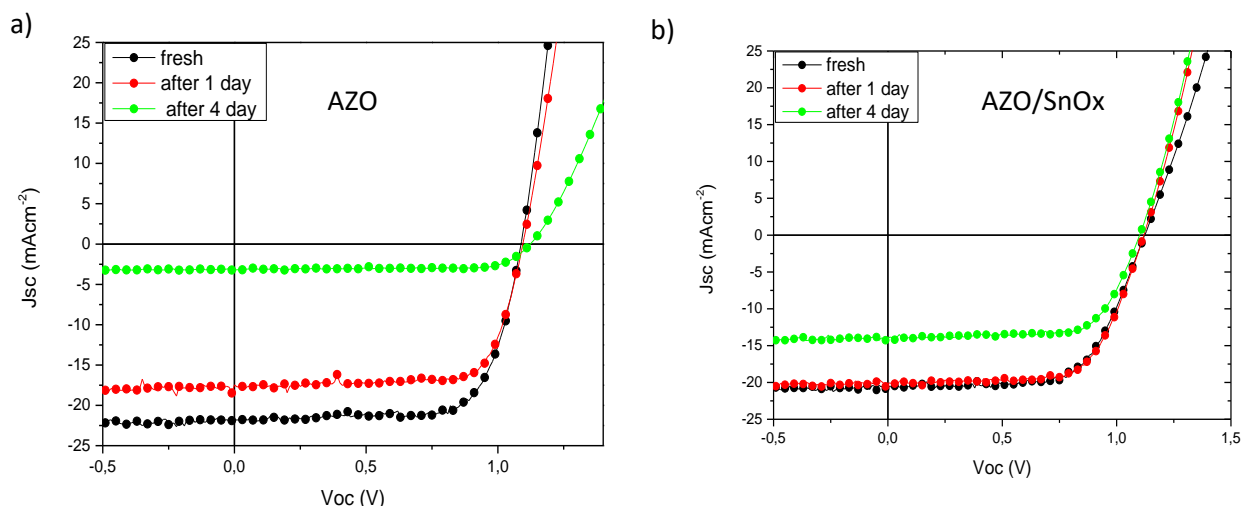


10-rasm: Azot(N) muhitida va vakuum(V) sharoitida 60°C(heated) da saqlanganda quyosh elementining barqarorligi.

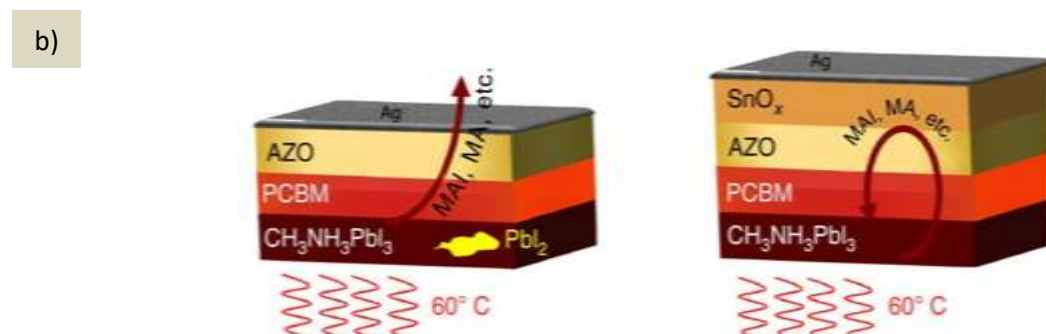
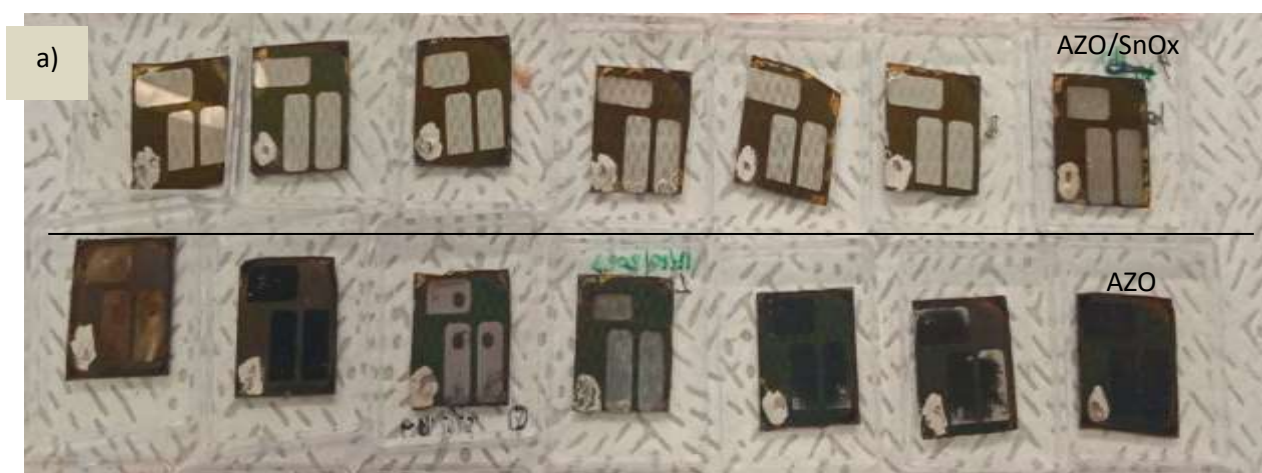
SnO_x qatlami mavjud bo'lmagan qurilmada samaradorlik keskin pasaydi: dastlabki(fresh) 17% dan 95 soat ichida 3% gacha tushib ketdi. Bu holat ion migratsiyasi, tuzilma degradatsiyasi va interfeysdagi nosozliklar bilan bog'liq bo'lishi mumkin.

Aksincha, SnO_x qatlami qo'shilgan qurilmada barqarorlik ancha yuqori bo'ldi: dastlabki 15% samaradorlik 50 soat davomida saqlanib, keyinchalik 11% gacha sekin kamaydi. Jsc qiymati ham barqaror saqlanib, fotozaryad tashish samaradorligi yuqori bo'lib qoldi.

SnO_x qatlami ion migratsiyasini cheklab, interfeysni himoya qiladi va elektron tashuvchi qatlam (ETL) vazifasini bajarib, uzoq muddatli ishlash barqarorligini ta'minlaydi. Eng muhimi, SnO_x qatlami bo'lgan qurilmalarda 12 kunlik qorong'i sharoitda saqlashdan keyin ishlash qobiliyatining qisman tiklanishi kuzatilgan. Bu esa, SnO_x ning nafaqat ishlash vaqtida barqarorlikni oshirishi, balki stressdan keyingi tiklanish mexanizmlariga ham yordam berishidan dalolat beradi. Aksincha, SnO_xsiz namunalarda hech qanday tiklanish kuzatilmagan, bu esa ulardagi degradatsiyaning qaytmas ekanligini anglatadi. Yakuniy xulosada, SnO_x qatlamining kumush (Ag) elektrodining korroziyasini (rang o'zgarishi) samarali ravishda oldini olishi vizual ravishda isbotlangan (**12-rasm**).



11-rasm. a) MAPbI₃ qurilmasining yorug‘lik (LED, 520 nm / P = 20 mW/cm²) ostida 10⁻⁴ mbar qattiq vakuum sharoitida 4 kun davomida ishlaganda o‘lchangan J–V xarakteristikasi. Qurilma tuzilishi: ITO/PTAA/MAPbI₃/PCBM/AZO(SnO_x)/Ag. **b)** Yuqori vakuum (10⁻⁴ mbar) sharoitida ishlaganda, ichki SnO_x to‘siq qatlami bilan va usiz MAPbI₃ perovskitli quyosh elementining quvvatni aylantirish samaradorligi (PCE) taqqoslanishi.



12-rasm. a) Yuqori vakuum sharoitida (10⁻⁴ mbar; 60 °C) termal stress ta‘sirida metall elektrodning korroziyasi tufayli yuzaga kelgan rang o‘zgarishini ko‘rsatadigan suratlar. MAPbI₃ qurilmasi SnO_x qatlami bilan va usiz taqqoslangan. **b)** ALD usulida o‘stirilgan ichki SnO_x to‘siq qatlamini qo‘shish orqali degradatsiya yo‘llarining bostirilishini ko‘rsatuvchi sxematik tasvir (Kai B va hammualliflar).

Bu SnO_x ning ionik va kimyoviy to‘siq sifatida ikki tomonlama funksiyani bajarishini tasdiqlaydi, ya‘ni perovskitdan ajralib chiqadigan halid ionlarining Ag elektrodiga yetib borishini to‘xtatadi. Bu esa qurilmaning strukturaviy yaxlitligini

saqlab qolishga yordam beradi. Tadqiqot natijalari SnO_x kabi oraliq qatlamlarning PQElarining uzoq muddatli chidamliligi uchun naqadar muhimligini namoyish etadi va kelajak avlod perovskit fotovoltaiq qurilmalarini yaratishda interfeys muhandisligi yo‘nalishiga qimmatli hissa qo‘shadi.

XULOSA

“Perovskit yutuvchi qatlamining shakllanish xususiyatlari bilan unga asoslangan quyosh elementlarining konversiya ko‘rsatkichlari o‘rtasidagi bog‘liqlik” mavzusida falsafa doktori (PhD) dissertatsiyasi bo‘yicha olib borilgan tadqiqotlar natijasida quyidagi xulosalar taqdim etildi:

1. Perovskit materiallarining shakllanish jarayonlari va ularni barqaror ishlashini ta‘minlaydigan omillar tadqiq etildi. Aniqlanishicha, poliyodid perovskitga o‘xshash tuzilmalar erituvchi turidan qat‘i nazar, prekursor eritmasi konsentratsiyasi ortishi bilan barqaror o‘sadi. Poliyodid komplekslarida zaryad/hajm nisbati kamaishi prekursor konsentratsiya oshgani sayin perovskitga o‘xshash tuzilmalar kattalashishiga olib keladi. Bu jarayon ^{207}Pb YaMR, UB, UPS va eritma o‘tkazuvchanligini baholash usullari orqali tasdiqlandi.

2. Ilk bora tiomochevina qo‘shimchasining ta‘siri ham o‘rganildi. U spin-coating bosqichida emas, balki asosan termik ishlov jarayonida namoyon bo‘lib, kristallarning $\langle 110 \rangle$ yo‘nalishi bo‘yicha o‘sishi va qayta yo‘nalishiga yordam beradi. Tiomochevina bo‘lmagan tizimlarda bunday ta‘sir kuzatilmadi. YaMR va UPS tadqiqotlari bu jarayonning mohiyati kristallarning tezroq o‘sishiga yordam beruvchi ionlarning yuqori harakatchanligi bilan bog‘liq ekanini ko‘rsatdi.

3. Tadqiqotlar natijasida p-i-n tuzilishga ega quyosh elementlari yaratildi. Ular 12 % dan 18 % gacha yetuvchi barqaror samaradorlikni namoyish etdi. Olingan ma‘lumotlar quyosh elementlarining chiqish xususiyatlari ularning morfologiyasi bilan chambarchas bog‘liqligini isbotladi. Bu bog‘liqlik tiomochevina ishtirokida shakllanadigan oraliq komplekslar, ularning rivojlanishi va termik ishlov jarayonida ionlar migratsiyasi kuchayishi bilan izohlanadi.

4. Gaz bilan sovutish qo‘shimchasi antesolventga nisbatan perovskit fazasining morfologiyasini shakllantirishda samaraliroq ekani aniqlandi. U polikristallarning bir necha yuz nanometr gacha o‘sishiga yordam beradi va natijada perovskitning optoelektron xususiyatlari yaxshilanadi. Bu yondashuv sanoat miqyosida qo‘llash va modul qurilmalar yaratishda ham qo‘llanishi mumkin.

5. Interfeys muhandisligi barqarorlik uchun hal qiluvchi ekanligi isbotlandi: Yuqori vakuum sharoitida o‘tkazilgan termik stress sinovlari interfeys muhandisligining PQElarining barqarorligi uchun hal qiluvchi rol o‘ynashini tasdiqladi. Ikki qatlamli AZO/ SnO_x elektron ekstraksiya qatlami (EEL) bo‘lgan ultra-barqaror invertirlangan arxitektura ishlab chiqildi. Bu yerda 20 nm qalinlikdagi ALD (atom qatlami bilan qoplash) usulida o‘stirilgan SnO_x qatlami zich to‘siq vazifasini bajarib, namlikning kirishini to‘xtatdi va parchalanish mahsulotlari, masalan, $\text{CH}_3\text{NH}_3\text{I}$ va HI ning chiqib ketishiga yo‘l qo‘ymadi. Bundan tashqari, bu qatlam ion migratsiyasi tufayli kelib chiqadigan degradatsiyani va elektrodning yemirilishini kamaytirib, o‘zining ko‘p funksiyali samaradorligini isbotladi.

**ONE-TIME SCIENTIFIC COUNCIL AT THE SCIENTIFIC COUNCIL
ON AWARD OF SCIENTIFIC DEGREES DSc.02/30.12.2019.K/FM/T.36.01
AT THE INSTITUTE OF POLYMER CHEMISTRY AND PHYSICS**

INSTITUTE OF POLYMER CHEMISTRY AND PHYSICS

JULLIEV ZAVKIDDIN NORMENGLI UGLI

**RELATIONSHIP BETWEEN THE FORMATION FEATURES OF A
PEROVSKITE ABSORBER AND THE CONVERSION PERFORMANCE OF
SOLAR CELLS BASED ON IT**

01.04.06 – Polymer physics

02.00.12 – Nanochemistry, nanophysics and nanotechnology

**DISSERTATION ABSTRACT OF THE DOCTOR
OF PHILOSOPHY (PhD) ON PHYSICAL – MATHEMATICAL SCIENCES**

Tashkent – 2025

The theme of the doctor of philosophy (PhD) is registered at the Supreme Attestation Commission under the Cabinet of Ministers of the Republic of Uzbekistan № B2025.2.PhD/FM1331.

The dissertation was carried out at the Institute of Polymer Chemistry and Physics.

The abstract of the dissertation in three languages (Uzbek, Russian, English (resume)) is available online (polchemphys.uz) and on the website of “ZiyoNET” information-educational portal (www.ziynet.uz).

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Leading organization: **Nanotechnology Development Center at the National University of Uzbekistan named after MirzoUlugbek**

The defense of the dissertation will take place on «__» january 2026 at «__» o'clock at a meeting of Scientific council DSc.02/30.12.2019.K/FM/T.36.01 at the Institute of Polymer Chemistry and Physics (Address: 100128, Tashkent city, Abdulla Kadiry str., 7^b, Ph.: (998-71) 241-85-94; fax: (998-71) 241-26-61; e-mail: polymer@academy.uz).

The dissertation can be reviewed at the Informational Resource Centre of Institute of Polymer Chemistry and Physics (registration number____ (Address: 100128, Tashkent city, Abdulla Kadiry str., 7^b, Ph.: (998-71) 241-85-94;).

The abstract of the dissertation has been distributed on «__» december 2025 y.

(Protocol at the register № _____ dated «__» december 2025 y).

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INTRODUCTION (PhD dissertation abstract)

Relevance and necessity of the dissertation topic. Due to the growth of the world's population, the demand for energy resources is rapidly increasing on a global scale. In this context, the creation of low-cost perovskite solar cells with simple production technology and high efficiency is one of the urgent challenges.

Currently, leading scientific centers worldwide are actively conducting research to address several critical issues facing perovskite-based solar cells in order to achieve high efficiency. In this regard, enhancing the optoelectronic properties of perovskite, finding ways to passivate and reduce defects, and improving the stability of devices are of great scientific importance.

In our Republic, consistent fundamental and applied research on alternative solar cells has also been carried out in recent years. Specifically, significant results have been achieved in the initial steps towards improving the conversion efficiency in PSCs, primarily by introducing specific additives into the active layer to find optimal conditions, understand their role, and study the stability of the resulting cells. These advancements primarily focus on identifying optimal conditions through the incorporation of specialized additives into the active layer, elucidating their underlying roles, and investigating the long-term stability of the resulting devices. Such research demonstrates that various specialized additives facilitate an increase in the final grain size of the perovskite active layer, thereby enabling the development of high-efficiency photovoltaic devices by reducing grain boundary density. Furthermore, the Development Strategy of New Uzbekistan and the Science Development Concept until 2030 outline clear objectives for “expanding and supporting the utilization of renewable energy sources”. In this regard, scientific and practical research aimed at the creation and practical implementation of a new generation of renewable solar cells remains of vital importance.

This dissertation research is aimed at solving the scientific and technical problems stipulated by the Law of the Republic of Uzbekistan dated May 21, 2019 No. LRU-539 "On the Use of Renewable Energy Sources," Resolution of the President of the Republic of Uzbekistan dated August 22, 2019 No. PD-4422 "On Accelerated Measures to Increase Energy Efficiency of the Economic and Social Spheres, Introduce Energy-Saving Technologies and Develop Renewable Energy Sources." This dissertation research, to a certain extent, serves the implementation of the tasks defined in the Resolution of the Cabinet of Ministers of the Republic of Uzbekistan "On the Use of Alternative Energy," as well as in other regulatory legal acts related to the use of alternative energy.

The Compliance of the research with the priority directions of development of science and technology of the Republic. This dissertation work was carried out in accordance with the priority areas of the development of science and technology of the Republic of Uzbekistan: III "Energy, energy efficiency, transport, development of mechanical and electronic equipment", II "Physics, astronomy, energy and mechanical engineering" and VII. "Chemical technologies and nanotechnologies".

The degree of study of the problem. In many leading scientific centers of the world, scientific research is being actively conducted to achieve high efficiency in solar cells based on perovskite. Park N.G., Snaith H.J. and a number of scientists have made a significant contribution to the development of scientific directions on

perovskite solar cells (PCE) with a planar structure. In many countries of the world, scientific research is being conducted aimed at improving the crystalline quality, granule growth, and stability of perovskite. In this direction, it is necessary to note the scientific research conducted by Yang Yang, J. Hou, and A. Hagfeldt on controlling the crystallization process using additives, by A. Graetzel, M. Saliba, and H. J. Snaith on morphology optimization and obtaining high-quality layers, and by Y. L. Loo, S. R. Forrest, and M. Graetzel on interface engineering in p-i-n structures to ensure long-term stability of PQE.

Academician S.Sh. Rashidova, Professors N. R. Ashurov's team, as well as B. L. Oksengendler, N. N. Turaeva, D. U. Matrasulov, E. Zakhidov, A. Zakhidov, and others, with their scientific research on organic-inorganic perovskites, have contributed to the development of this area in our republic.

Until this study, there was no sufficient scientific basis in the literature for a deep study of the mechanisms of formation of the morphology of the perovskite layer, which is one of the main factors determining the efficiency of PQEs, in particular, to reveal the exact mechanism of the effect of special additives on crystal growth. This limits the ability to stably control the crystallization process of the active layer and ensure the repeatability of the device efficiency. In addition, there is a lack of systematic studies on the optimal morphology, optoelectronic properties and long-term stability of p-i-n PQEs under various external factors. Therefore, it is necessary to conduct in-depth fundamental and scientific-practical research in this area to create highly efficient and stable PQEs and eliminate the main problems encountered in practical applications.

The connection of the investigation with plans of science-investigate works of the science-investigate institution where the dissertation was carried out. The dissertation research was conducted as part of the basic research plan of the Institute of Polymer Chemistry and Physics of the Academy of Sciences of the Republic of Uzbekistan (2020-2024), as well as within the framework of the fundamental project REP-24112021/33 "Perovskite solar cells with optimized performance and stability" (2022-2024).

The aim of the study is to investigate the kinetics of perovskite absorber formation from precursor solutions in relation to their morphology, and to determine the role of a specific additive (thiourea) in promoting polycrystal grain growth, as well as its correlation with the efficiency and stability characteristics of inverted perovskite solar cells.

Research Tasks:

to investigate the dependence of intermediate complex formation on the precursor concentration in various solvents, and to identify the structural parameters responsible for the morphological development of the perovskite absorber.

to determine the role of the special additive, thiourea (as a Lewis base), at all stages of perovskite absorber formation (spin-coating, gas quenching, antisolvent treatment, and thermal annealing).

to perform a comparative evaluation of the dynamics of perovskite absorber morphological development using spin-coating approaches, specifically the gas quenching and antisolvent methods.

to create inverted solar cells with optimal morphological and optoelectronic properties and to determine the correlation between these properties and their conversion efficiency.

to test the stability of p-i-n structured perovskite solar cells under various conditions, with the specific goal of enhancing device stability through interface engineering.

Object of the Study. The research focuses on MAPbI₃ perovskite active layers, PTAA polymer semiconductor serving as the hole transport layer, the thiourea additive as a crystallization modifier (Lewis base), and SnO_x electron transport layers, as well as the solar cells fabricated based on these components.

Subject of the Study. The subject of this research includes colloidal lead complexes present in the precursor ink, as well as the grain size and crystal structure of MAPbI₃ perovskites modified with a specific additive. It also encompasses the optical, optoelectronic, photovoltaic, and stability properties of solar cells fabricated with the ITO/PTAA/MAPbI₃/PCBM/AZO/(SnO_x)/Ag device architecture.

Research Methods. In the preparation of perovskite solar cells, several fabrication and processing techniques were employed, including spin-coating, anti-solvent treatment, gas quenching, surface modification, structural modification, and thermal annealing. The crystal lattice structure and morphology of perovskite films were analyzed using X-ray diffraction (XRD), grazing-incidence wide-angle X-ray scattering (GIWAXS), scanning electron microscopy (SEM), atomic force microscopy (AFM), and nuclear magnetic resonance (NMR) spectroscopy. The optical and electronic properties of the samples were studied using UV-Vis and in situ UV-Vis absorption spectroscopy, steady-state and time-resolved photoluminescence (PL), Raman spectroscopy, ultraviolet photoelectron spectroscopy (UPS), and X-ray photoelectron spectroscopy (XPS). Device performance parameters such as current-voltage (J-V) characteristics, electrochemical impedance spectroscopy (EIS), hysteresis factor, defect density, and density of defect energy states—were determined through electrical measurements. Finally, stability tests were conducted under controlled conditions using maximum power point tracking and other standardized testing protocols to evaluate long-term operational durability.

Scientific novelty of the dissertation research.

for the first time, the growth mechanism of polyiodide complexes during the formation of the perovskite absorber was elucidated, showing that their evolution is governed by precursor concentration regardless of the solvent type.

the role of thiourea additives in the perovskite crystallization process was identified for the first time. It was revealed that thiourea becomes primarily active during thermal annealing, promoting crystal growth and reorientation along the <110> direction—an effect associated with increased ionic mobility.

a stable MAPbI₃-based p-i-n solar cell was developed using a bilayer AZO/SnO_x electron extraction layer (EEL). The SnO_x layer was found to act as a multifunctional barrier that effectively suppresses ion migration and electrode corrosion.

The practical results of the research are as follows:

a unified growth pattern of polyiodide perovskite-like structures was determined to be independent of solvent type or mixture, emerging with increasing

precursor concentration. This conclusion was quantitatively confirmed through ^{207}Pb NMR, UV-Vis, UPS, and conductivity measurements. The analyses reveal a decrease in the charge-to-volume ratio of polyiodide complexes at higher precursor concentrations, consistent with the growth of perovskite-like structures.

for the first time, a comprehensive understanding of the structural evolution of the perovskite absorber in the presence of the additive thiourea has been developed, encompassing both the precursor solution spin-coating stage and the crystallization during thermal annealing. In situ GIWAXS measurements reveal that polyiodide complex formation is a dynamic process initiated at the spin-coating stage, while the specific influence of thiourea emerges during annealing, where it drives crystal reorientation and promotes growth along the $\langle 110 \rangle$ plane—a behavior not observed without the additive.

complementary NMR and UPS studies further indicate that this effect is linked to enhanced ionic mobility, likely originating from the high mobility of thiourea molecules under thermal conditions. Taken together, these results provide a consistent mechanism by which thiourea facilitates crystal growth, and this mechanism has been determined.

it was revealed that GQ is more effective than the antisolvent in controlling the perovskite phase morphology, enabling the growth of polycrystals up to several hundred nanometers. Such morphology development improves the optoelectronic properties of perovskite, and the scalability of this approach for industrial device fabrication has been determined.

inverted solar cells with a p-i-n structure was fabricated, showing reproducible efficiencies ranging from 12% to over 16%. The correlation between morphological parameters and device performance, arising from thiourea-induced intermediate complex formation and crystal growth during thermal treatment through ion migration channels, has been determined.

the thermal stress test under high vacuum conditions confirmed the crucial role of interfacial engineering in perovskite solar cells. Incorporation of a SnO_x layer effectively suppressed Ag electrode corrosion, thereby improving both physical and electrical durability. An ultra-stable inverted architecture with a bilayered AZO/ SnO_x electron extraction layer (EEL) was developed, where the 20 nm ALD-grown SnO_x acted as a dense permeation barrier, blocking moisture ingress and preventing the release of decomposition products such as $\text{CH}_3\text{NH}_3\text{I}$ and HI. This layer also reduced degradation and inhibited electrode erosion caused by ion migration, and its multifunctional effectiveness has been determined.

Reliability of research results. In the dissertation work, more than 10 modern research methods were used to determine all parameters of the perovskite solar cell. Structural, optical, electronic, photovoltaic, and stability the results of his research confirm each other. For the analysis of quantities of a random nature, 10 units were manufactured from each type of device, and their parameters were measured under the same conditions. The obtained scientific and practical results were discussed at a number of republican and international scientific conferences.

Scientific and Practical Significance of the Research Results. The scientific significance of the research results is that the universality of the concentration-dependent growth pattern of polyiodide complexes in the formation of perovskite absorbers and their independence from the type of solvent were quantitatively

confirmed by experimental methods (^{207}Pb NMR, UV-Vis, UPS, conductivity measurements). The role of the thiourea additive in the dynamics of perovskite crystallization was determined; it was proven that it is activated during thermal treatment and stimulates the reorientation and growth of crystals in the $\langle 110 \rangle$ direction, and this effect is associated with the high mobility of ions.

The practical significance of the research results is that more stable and highly efficient PSC with the ITO/PTAA/MAPbI₃/PCBM/AZO/(SnO_x)/Ag structure, developed based on a two-layer AZO/SnO_x electron extraction layer, are resistant to thermal stress under high vacuum conditions, and the SnO_x layer effectively suppresses electrode corrosion by preventing the ingress of moisture and decomposition products, and the possibility of extending the device's operating life has been investigated.

Implementation of Research Results. Based on the scientific results obtained on the topic “Relationship between the formation features of a perovskite absorber and the conversion performance of solar cells based on it”:

by introducing special additives (additive) such as thiourea into the active layer and showing a dense barrier with a SnO_x layer grown on top of the active layer, it was used in the implementation of the fundamental project No. IL-5421101892 "Study of the fundamental foundations of the luminescence properties of energy-saving structures based on semiconductor perovskites," carried out at the S.A. Azimov Physical-Technical Institute of the Academy of Sciences of the Republic of Uzbekistan (certificate No. 01/467 dated September 8, 2025). It has been established that the size of crystallites (grains) in the active layer of CsPbBr₃ is increased by the introduction of special additives (additive) such as thiourea (SC (NH₂)₂), which were successfully used. In photosensitive devices based on the SnO_x electron extraction layer (EEL) architecture CsPbBr₃, long-term operational stability of the devices has been achieved.

the findings of the dissertation were successfully implemented within the framework of the international project “Light Harvesting in Space with Perovskite Solar Cells (SpacePerCells)”, funded by the NATO Science for Peace and Security (SPS) Programme. This project is a high-level collaboration between the Wuppertal Center for Smart Materials & Systems (Wuppertal, Germany) and the Institute of Polymer Chemistry and Physics (Tashkent, Uzbekistan). The research established that the AZO/SnO_x dual-layer electron extraction layer (EEL), integrated into the ITO/PTAA/MAPbI₃/PCBM/EEL/Ag device architecture, significantly enhances the long-term operational stability and structural durability of the solar cells. Specifically, this dual-layer EEL functions as an effective permeation barrier, mitigating the migration of mobile ions from the perovskite lattice and preventing the egress of volatile halide species. These findings proved critical for maintaining functional performance under low-pressure (vacuum) conditions, which are characteristic of space environments. (Confirmed by: Recommendation letter from the Professor of the University of Wuppertal and the international project certification)

Approval of Research Results. The main findings of the dissertation have been presented and discussed at 2 international and 4 national scientific-practical conferences. These platforms served as forums for peer review and expert feedback, contributing to the refinement and validation of the research outcomes.

Publication of Research Results. A total of 10 scientific papers have been published on the topic of the dissertation. Among these, 5 scientific articles were published in journals recommended by the Higher Attestation Commission of the Republic of Uzbekistan for publishing the main scientific results of doctoral (PhD) dissertations. Specifically, 3 of these articles were published in national journals and 2 in international journals.

Structure and Scope of the Dissertation. The dissertation consists of an introduction, four main chapters, a conclusion, a list of references, and appendices. The total volume of the dissertation is 102 pages.

MAIN CONTENT OF THE DISSERTATION

The introduction substantiates the relevance and demand for the topic of the dissertation, formulates the purpose and objectives of the study, identifies the objects and subject of the study, shows the compliance of the study with the priority areas of development of science and technology of the Republic of Uzbekistan, presents the scientific novelty and practical results of the study, substantiates the reliability and reveals the scientific and practical significance of the results obtained, formulates conclusions, notes the prospects for the implementation of the research results in practice, and provides information on published works and the structure of the dissertation.

The first chapter of the dissertation entitled "**The current state of the problem of obtaining high-quality perovskite films, the development of solar cells, and stabilization strategies**" provides a detailed explanation of the formation of perovskite thin films, specifically the complexities of the solution-processing stage, the mechanisms of crystal nucleation and growth, and the influence of the precursor solution. Furthermore, it presents a literature review dedicated to examining the effects of key technological processes like **spin-coating** and **thermal annealing** on the quality of perovskite films, their theoretical foundations, and the role of additives in controlling crystal grain size, orientation, and defects. The chapter emphasizes the need for a deeper understanding of the connection between solution chemistry, the coating process, and the transition to the solid phase to achieve consistent and reproducible results for perovskite devices.

The second chapter of the dissertation, titled "**Research Objects and Methods**" provides a detailed description of the procedures and techniques used for the fabrication and characterization of perovskite solar cells. The chapter explains the device structure, the function of each layer (including SnO₂, the perovskite active layer and the silver top electrode), and the specific processes for their preparation. It also summarizes the instruments and methods used for optical, crystallographic, morphological, rheological, and electrophysical characterization, such as UV-Vis, XRD, AFM, FTIR, SEM, and a 4-probe setup. The evaluation of device efficiency and photovoltaic parameters through I-V and IS measurements under a solar simulator is also discussed.

The third chapter of the dissertation, titled "**Lewis Base-Mediated Crystallization Control in Inverted Perovskite Solar Cells Using Thiourea Additive,**" provides an in-depth study of the processes involved in the formation of the perovskite active layer. The main objective of the chapter is to determine the

influence of specific additives, particularly thiourea ($\text{NH}_2\text{-CS-NH}_2$), on the crystallization, morphology, and optoelectronic properties of perovskite films prepared using spin-coating and thermal annealing methods.

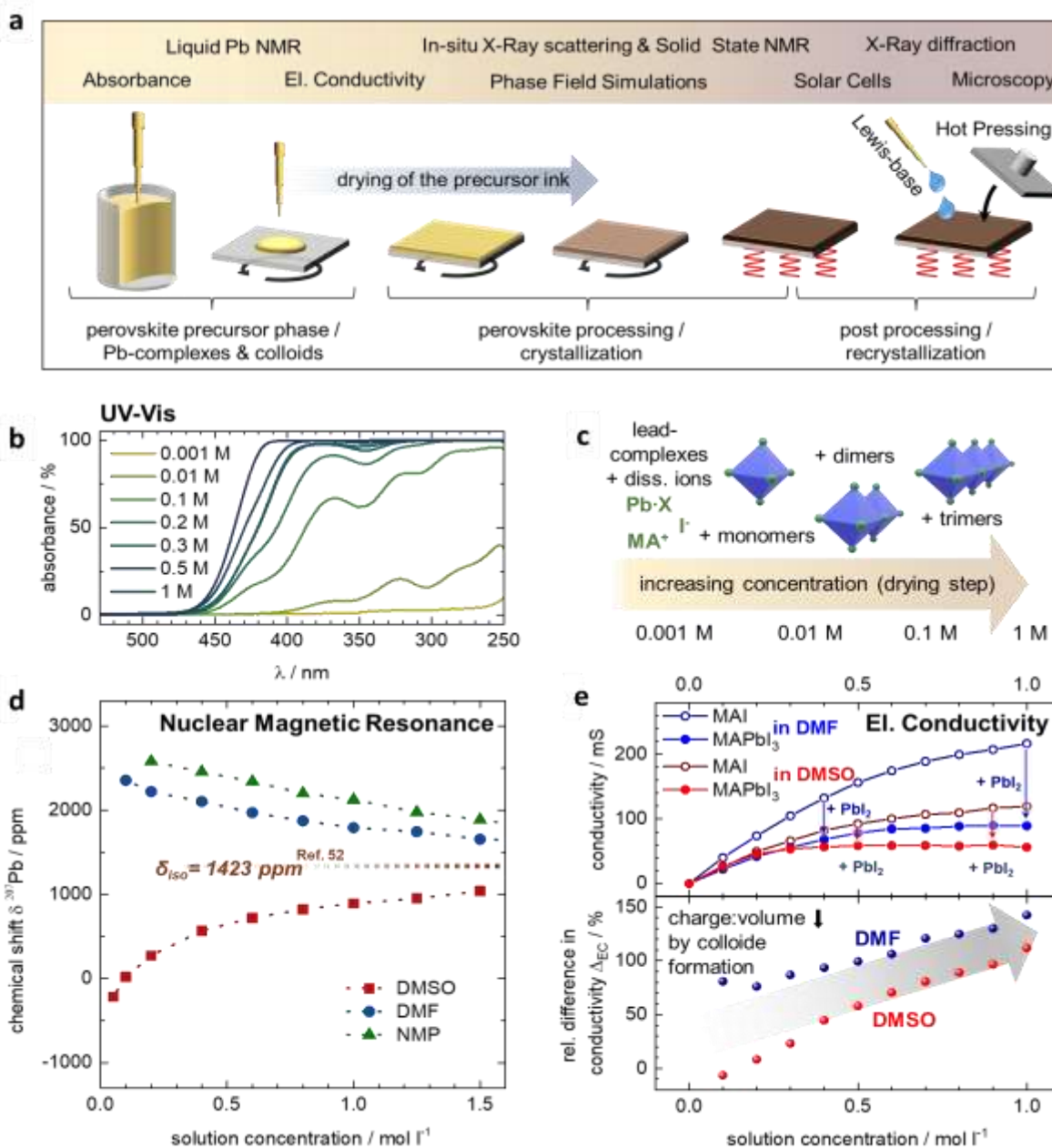


Figure 1. Solvent chemistry (type and concentration): a) Schematic of perovskite deposition and measurement methods. b) UV-Vis absorbance of MAPbI₃ inks in DMF at varying concentrations. c) Illustration of lead complex evolution with concentration. d) ²⁰⁷Pb NMR of MAPbI₃ inks in DMF, DMSO, and NMP vs precursor molarity; dotted line marks solid-state MAPbI₃. e) Conductance comparison of MAPbI₃ vs MAI in DMF, DMSO, and NMP at different concentrations; lower panel shows relative conductance difference (Δ_{EC}).

These complexes delay perovskite crystallization, allowing for better control over the thin film's quality. The study used three different solvents with varying donor properties: DMF, DMSO, and NMP. The properties of the resulting polycomplexes were investigated as a function of solution concentration using UV-Vis spectroscopy, ²⁰⁷Pb NMR spectroscopy, and conductivity measurements (**Figure**

1). The results indicate that as the solution concentration increases, the volume of the polyiodide complexes grows, leading to a decrease in the charge-to-volume ratio.

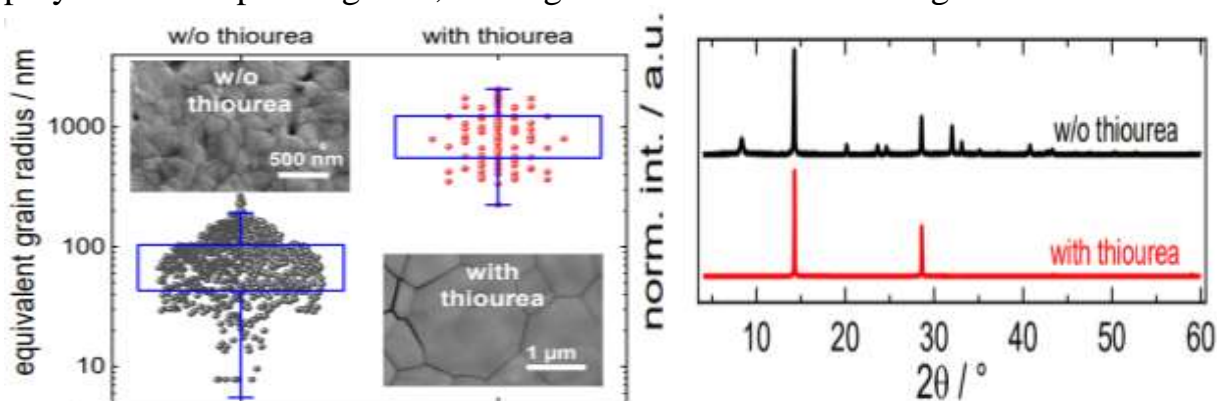


Figure 2: Impact of thiourea additive. a) Grain size distribution and SEM images of MAPbI₃ layers deposited from an DMF:NMP precursor ink by gas quenching with a concentration of 1.0 M with and w/o 0.1 M of thiourea additive (left). b) XRD patterns of respective layers with and without 0.1 M thiourea (right).

A crucial part of the research involved adding a thiourea additive to the perovskite solution to study its effect. As a neutral molecule, thiourea does not disrupt the ionic equilibrium in the solution, which makes it an effective additive. Experimental results show that the presence of thiourea significantly increases the size of perovskite grains, leading to a reduction in defects and an improvement in device stability (**Figure 2**). X-ray diffraction (XRD) and scanning electron microscopy (SEM) analyses confirmed that the grain size was larger in the samples containing the additive.

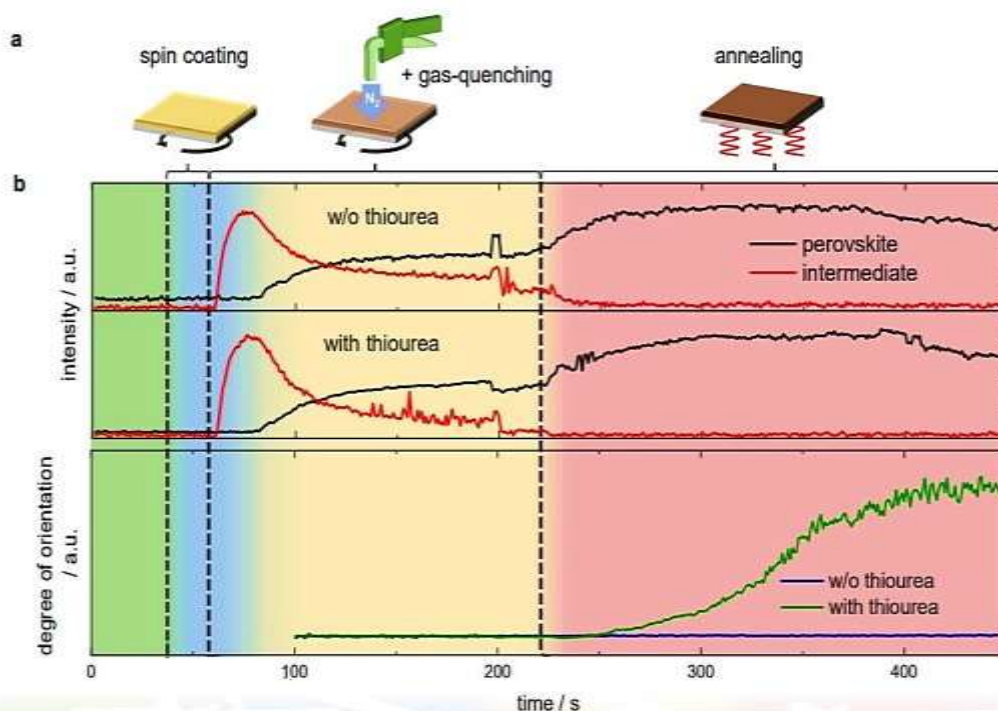


Figure 3: Perovskite formation process. a) Schematic of the in-situ deposition experiment. b) Time-dependent GIWAXS intensities of perovskite and the PbI₂•NMP intermediate, with and without thiourea, showing relative phase content.

Orientational order, given by the $90^\circ/45^\circ$ intensity ratio, indicates grain growth with preferential orientation, enhanced by thiourea (bottom) (**Figure 3**). All samples used a 7:3 DMF: NMP solvent mixture. Artefacts near 200 s arise from the end of spin-coating. To observe the evolution of the perovskite structure in real-time, advanced synchrotron techniques such as in situ GIWAXS (Grazing-Incidence Wide-Angle X-ray Scattering) were employed. The results of the study show that in samples containing the thiourea additive, the crystallites underwent significant reorientation during the thermal annealing stage, forming highly ordered perovskite domains. This behavior was not observed in the control samples.

The fourth chapter of the dissertation, titled "**Anti-Solvent and Gas-Quenching Methods for Controlled Crystallization of Active Layer in Perovskite Solar Cells,**" analyzes one of the central challenges in fabricating perovskite films: achieving precise control over the crystallization process. The chapter explores the widely used anti-solvent and gas-quenching methods for forming high-quality and long-term stable perovskite layers. While it has been effective, its manual application introduces variability and makes it impractical for large-scale production. These limitations highlight the need for new approaches to guarantee film quality and efficiency. This technique uses an inert gas (nitrogen or argon) to rapidly remove the solvent, thus controlling crystallization. Its key advantages include precise tunability (gas flow rate, quenching duration), the ability to produce uniform, smooth films with fewer defects, and its compatibility with large-scale manufacturing techniques like blade coating and slot-die coating. The main part of the chapter is dedicated to a comparative analysis of the effects of anti-solvent and gas-quenching techniques on the optical and structural properties of the films. Furthermore, UV-Vis spectroscopy analysis found that the films produced using gas quenching had a much more efficient light absorption across the entire UV-visible spectrum (**Figure 4**). In particular, the absorption coefficient at a wavelength of 550 nm exceeded 1.5, proving the superior light-harvesting capability of these films.

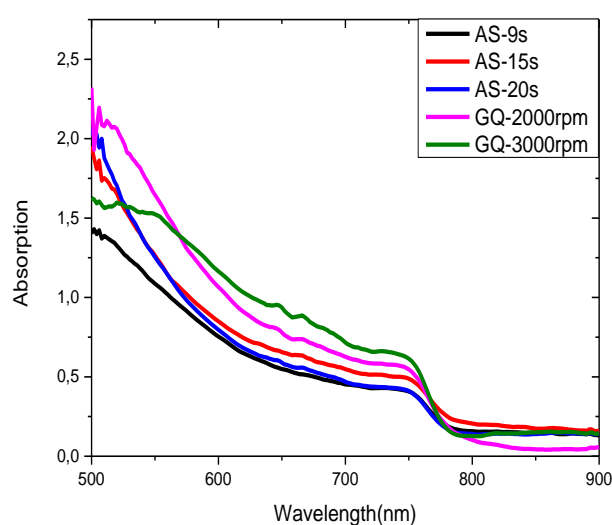


Figure 4. Absorption of ITO glass/PTAA/perovskite. Gas quenching (GQ) and Anti-solvent (AS).

Photoluminescence (PL) and Time-Resolved Photoluminescence (TRPL) measurements also demonstrated the superiority of the gas-quenching method. The PL intensity was significantly lower in gas-quenched samples, suggesting a more

efficient charge extraction process or reduced non-radiative recombination losses (**Figure 5**).

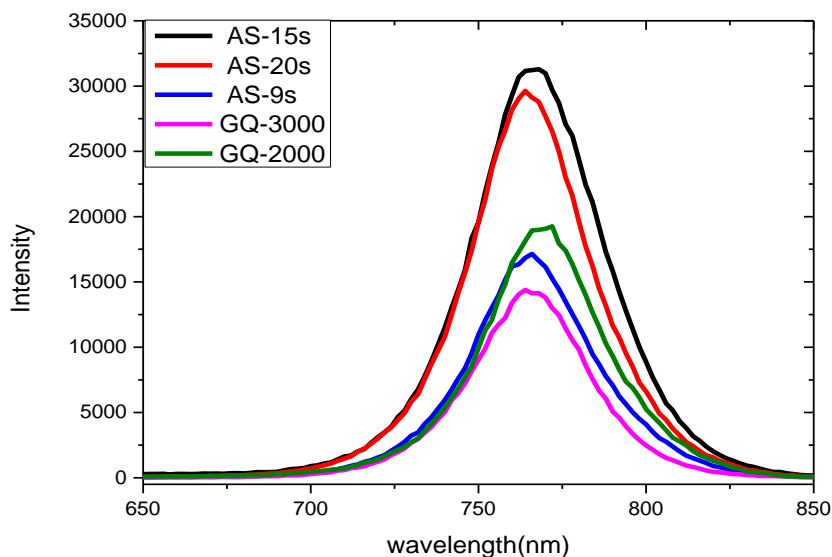


Figure 5. Steady-state photoluminescence (PL) of ITO glass/ PTAA/ MAPbI₃. Gas quenching (GQ) and Anti-solvent (AS).

TRPL analysis showed that the values for both the fast (τ_1) and slow (τ_2) decay components were optimized in the gas-quenched samples (**Figure 6**). This indicates a reduction in defect density and improved collection efficiency within the perovskite layer .

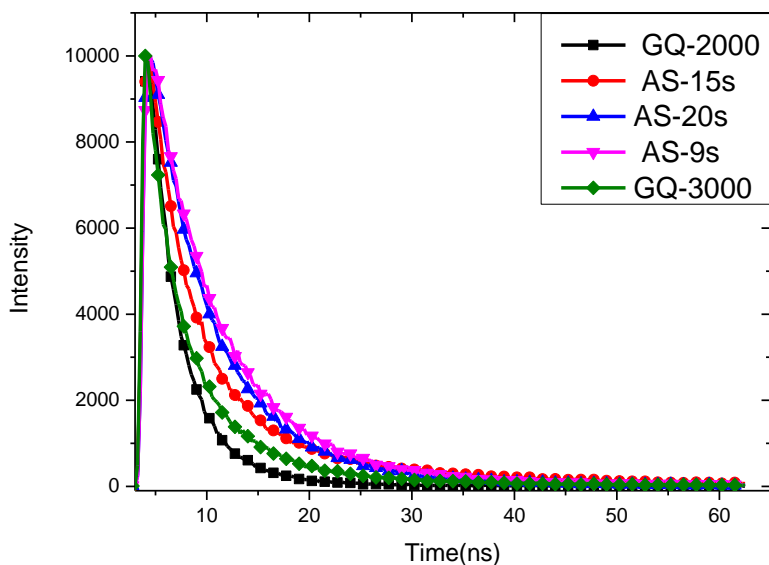


Figure 6. Time-resolved photoluminescence (TRPL) spectra of ITO glass/PTAA/perovskite. Gas quenching (GQ) and Anti-solvent (AS).

In conclusion, the research findings demonstrate that the gas-quenching method is more promising for shaping the morphology of the perovskite phase. This technique promotes the growth of polycrystals up to several hundred nanometers. The development of such morphologies improves the optoelectronic characteristics of perovskite, and the proposed approach is highly suitable for scaling and creating industrial prototypes of modular devices.

The **fifth chapter** of the dissertation, titled "**Creation of a solar cell based on a perovskite absorber (MAPb) in thiourea additive and GQ engineering,**" provides a detailed investigation into the fabrication and operational mechanisms of

high-efficiency inverted (p-i-n) perovskite solar cells. Building upon the results of previous research, this chapter focuses on significantly enhancing device performance by synergistically applying thiourea additives and gas-quenching technology. **The first part of the chapter** delves into the role of the thiourea additive as a Lewis base in the formation of perovskite crystals. The study, which used MAPbI₃ perovskite, identified two distinct mechanisms by which thiourea exerts its influence: First, as a Lewis base, it coordinates with lead ions (Pb²⁺), modulating the nucleation process. This slows down crystallization, promoting the formation of larger and more uniform grains. Second, the sulfur and nitrogen atoms in thiourea passivate defects within the layer, reducing trap-assisted recombination. According to the research results, samples with the thiourea additive achieved a high power conversion efficiency (PCE) of up to 16.83%, while control (additive-free) samples showed only 11.1% efficiency (**Figure 7**). These findings prove thiourea's crucial role as a Lewis base in improving the photovoltaic performance and film quality of perovskite.

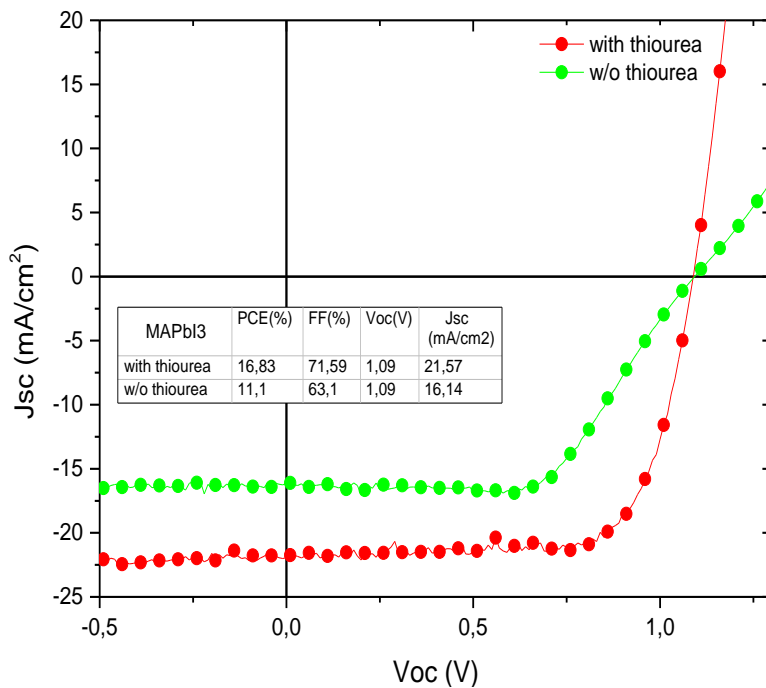


Figure 7. J-V character of inverted perovskite solar cell with and without thiourea.

The second part of the chapter determined the optimal concentration of the PTAA solution used as the hole transport layer (HTL) in p-i-n type perovskite solar cells. The J-V characteristics of devices were measured and compared using PTAA solutions at various concentrations (1.5-5 mg/ml). The results showed that at low PTAA concentrations, key parameters like Jsc, Voc, PCE, and FF had low values. This was attributed to a thin or incomplete HTL, which increased the device's series resistance. Conversely, as the concentration was increased (3-5 mg/ml), the fill factor (FF) significantly improved, indicating better contact between the HTL and the perovskite layer. The highest efficiency was observed at a concentration of 5 mg/ml, where the PCE reached 17.3%, with a Voc of 1.05 V, and a Jsc of 22 mAcm⁻²

(Figure 8). These results demonstrate that a higher-concentration PTAA solution forms a denser and better-connected film, ensuring higher mobility for hole carriers and more efficient charge collection.

In conclusion, the chapter describes the successful creation of inverted solar cells with a p-i-n structure using the thiourea additive and gas-quenching method. These devices demonstrated a reproducible high power conversion efficiency ranging from 12% to over 16%. The findings reliably prove a strong correlation between morphological parameters and the device's output characteristics. The mechanisms identified in the study such as the development of intermediate complexes and crystal growth during thermal treatment due to the opening of ion migration channels played a decisive role in enhancing overall device efficiency. This approach represents a simple and scalable solution for further improving the performance of perovskite photovoltaics through molecular-level engineering.

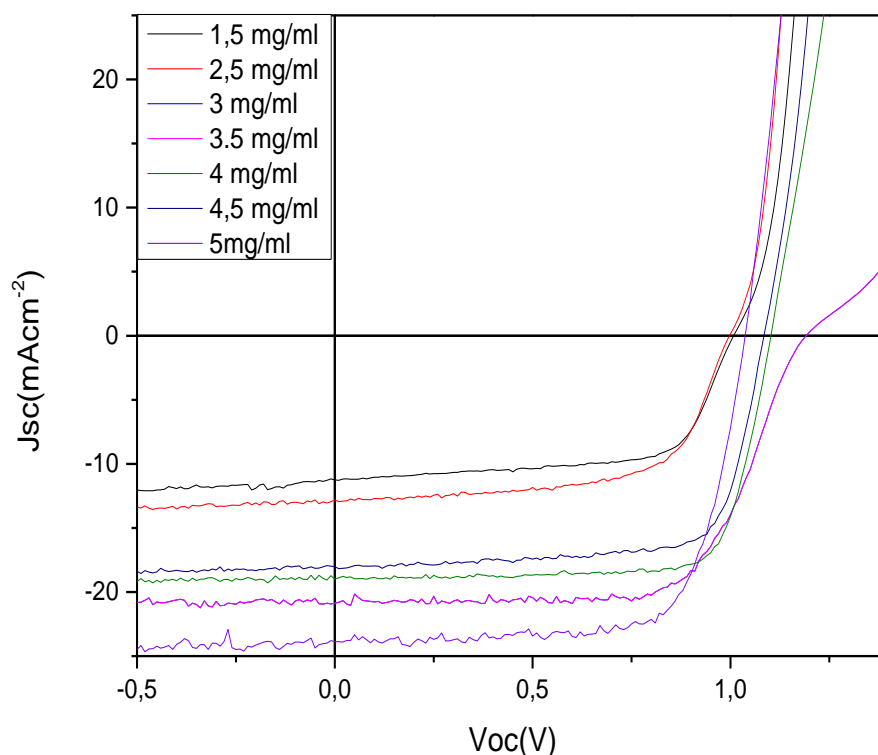


Figure 8: a) Statistical values of U_{oc} , J_{sc} , PCE, FF b) J-V characteristics of Perovskite solar cell with different concentration PTAA/Toluene 1.5 - 5 mg/ml.

The **sixth chapter** of the dissertation, titled "**Enhanced Stability in Inverted Perovskite Solar Cells via a Bilayered AZO/SnO_x Electron Extraction Interface,**" provides an in-depth study of operational stability, one of the most critical challenges hindering the commercialization of perovskite solar cells (PSCs). The main objective of the chapter is to systematically analyze the role of a SnO_x interlayer in enhancing the thermal, photostructural, and operational stability of MAPbI₃-based devices. This investigation is based on comprehensive testing conducted under high vacuum and continuous illumination conditions. The study fabricated devices with the ITO/PTAA/MAPbI₃/PCBM/AZO/(SnO_x)/Ag architecture

and tested their operational stability under high vacuum (10^{-4} mbar) and continuous illumination (520 nm LED, 20 mW/cm²). A dedicated section of the chapter explores the degradation mechanisms that occur under different conditions. The impact of moisture and oxygen on the perovskite material is analyzed. It is noted that in the presence of water vapor, the perovskite decomposes through reactions like $\text{CH}_3\text{NH}_3\text{PbI}_3 \rightarrow \text{CH}_3\text{NH}_3\text{I} + \text{PbI}_2$, leading to irreversible degradation. The degradation mechanism in a N₂ atmosphere is less damaging, primarily related to ion migration, and is shown to be partially reversible (**Figure 9**).

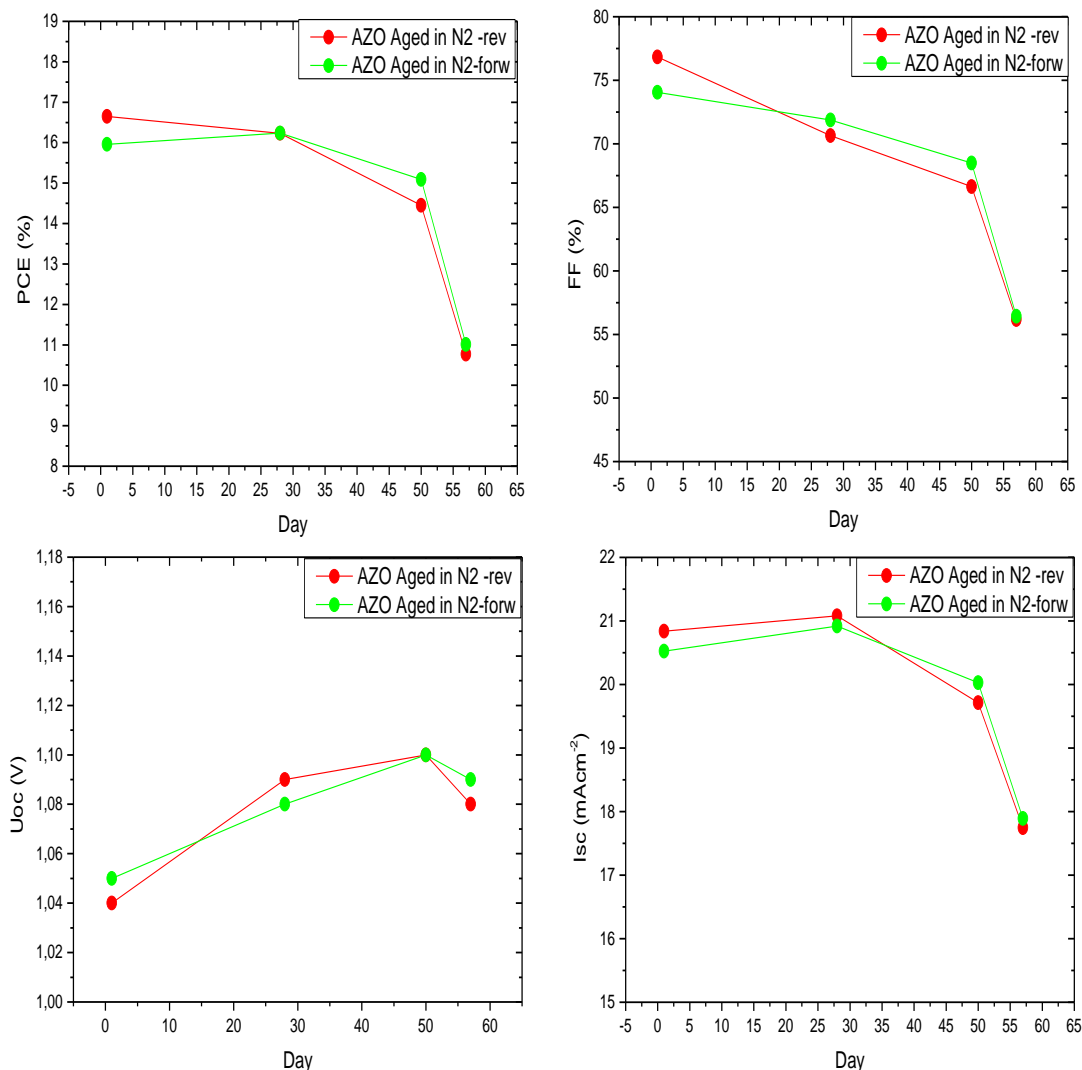


Figure 9: Stability of aged solar cell in nitrogen atmosphere

High-temperature stability tests were also of great importance. Tests conducted at 60°C showed that samples stored under vacuum degraded faster than those in a N₂ atmosphere (**Figure 10**). Under vacuum, the PCE dropped from 16% to 12%, whereas in an N₂ environment, it decreased by only about 0.5%. These results confirm that vacuum intensifies ion migration, causing the active layer to decompose. Furthermore, an extended analysis of J–V characteristics noted that the SnO_x layer acts as a protective buffer, effectively suppressing moisture ingress, ion migration, and interface deterioration. At **Figure 11**, Operational stability of MAPbI₃-based perovskite solar cells under high vacuum (10^{-4} mbar). The stability of MAPbI₃ perovskite solar cells with the architecture.

ITO/PTAA/MAPbI₃/PCBM/AZO/(SnO_x)/Ag was investigated under continuous illumination (LED, 520 nm, 20 mW/cm²) for 4 days. Devices with and without the SnO_x interlayer were compared. The device without SnO_x showed severe degradation: its PCE dropped sharply from 17% to 3% within 95 hours, indicating instability due to ion migration, structural degradation, and interfacial defects. In contrast, the SnO_x-containing device exhibited significantly improved stability. The initial PCE of 15% remained stable for 50 hours and gradually decreased to 11% after 95 hours. The J_{sc} values also remained stable, confirming efficient

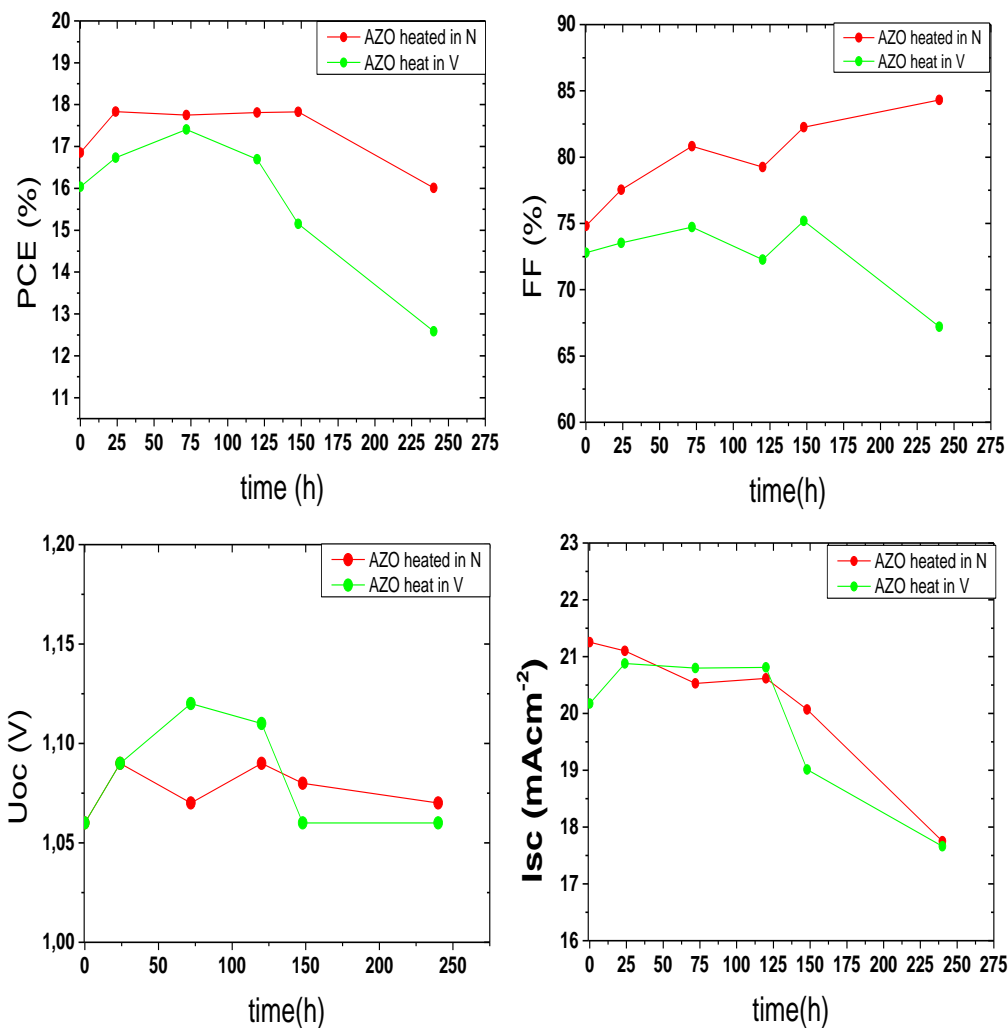


Figure 10: Stability upon storage at 60 °C in nitrogen atmosphere and vacuum condition.

charge generation and transport throughout the test. The SnO_x layer effectively suppresses ion migration, protects the interface, and functions as an efficient electron transport layer (ETL), thereby ensuring long-term operational stability. Most importantly, a partial recovery in performance was observed in devices with the SnO_x layer after a 12-day period of storage in the dark. This suggests that SnO_x not only enhances stability during operation but may also facilitate post-stress recovery mechanisms. In contrast, no recovery was observed in SnO_x-free samples, indicating that their degradation was irreversible. In conclusion, it was visually proven that the SnO_x layer effectively prevents the corrosion of the silver (Ag) electrode (discoloration) (**Figure 12a**). This confirms that SnO_x performs a dual function as

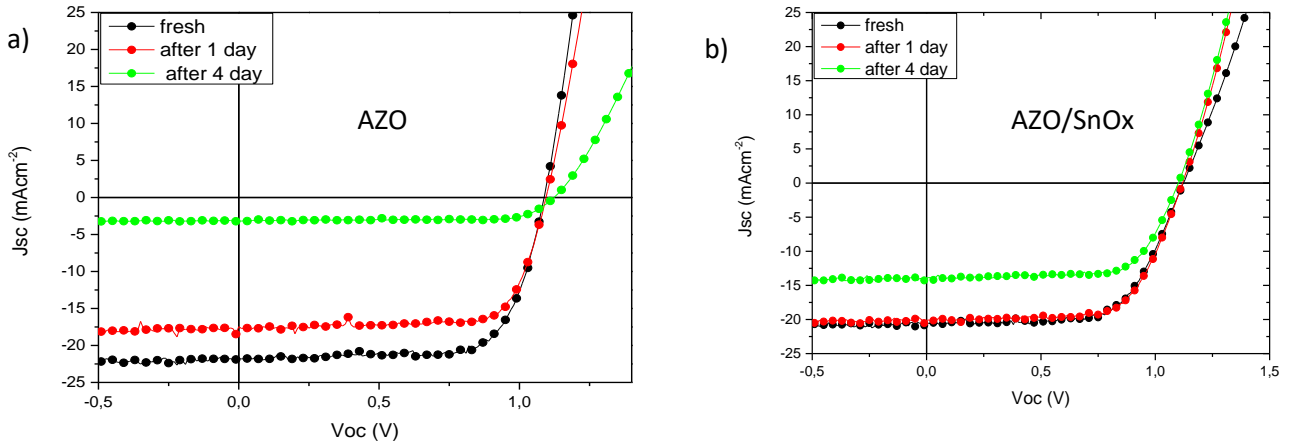


Figure 11: a) J-V characteristics of a MAPbI₃ device under operation with light (LED, 520nm/P=20mW/cm²) in harder vacuum conditions of 10⁻⁴ mbar for 4 days. ITO/PTAA/MAPbI₃/PCBM/AZO(SnOx)/Ag. b) Power conversion efficiencies of a MAPbI₃ perovskite solar cell with and without an internal SnOx barrier layer upon operation in high vacuum (10⁻⁴ mbar).

both an ionic and a chemical barrier, stopping halide ions from the perovskite from reaching the Ag electrode.



Figure 12: a) Photographs showing the colour change (the corrosion of metal electrode) upon thermal stress under the same high vacuum conditions (10⁻⁴ mbar; 60 °C). MAPbI₃ device with and without SnO_x. b) Schematic illustration depicting the suppression of degradation pathways through the incorporation of an ALD-grown internal SnO_x barrier.

This helps to maintain the structural integrity of the device. The results of the study demonstrate the critical importance of interlayers like SnO_x for the long-term durability of perovskite solar cells and contribute valuable insights to the field of interface engineering for next-generation perovskite photovoltaics.

CONCLUSION

As a result of the research conducted for the dissertation of Doctor of Philosophy (PhD) on the topic " Relationship between the formation features of a perovskite absorber and the conversion performance of solar cells based on it" the following conclusions were presented:

1. Polyiodide perovskite-like structures grow steadily as the precursor solution concentration increases, regardless of the type of solvent. A decrease in the charge-to-volume ratio within the polyiodide complexes leads to the enlargement of these perovskite-like structures as the precursor concentration rises. This process was confirmed using methods such as ^{207}Pb NMR, UV, UPS, and solution conductivity measurements.

2. For the first time, the effect of a thiourea additive was also studied. It was found to exert its influence mainly during the thermal annealing process, not the spin-coating stage. It promotes the growth and reorientation of crystals along the $\langle 110 \rangle$ direction. This effect was not observed in systems without thiourea. NMR and UPS studies showed that the essence of this process is related to the high mobility of ions, which helps the crystals grow faster.

3. The research led to the creation of p-i-n structured solar cells. They demonstrated stable efficiencies ranging from 12% to 18%. The data obtained proved that the output characteristics of the solar cells are closely linked to their morphology. This relationship is explained by the intermediate complexes formed in the presence of thiourea, their development, and the increased ion migration during the thermal annealing process.

4. It was found that the gas quenching method is more effective than antisolvent treatment for shaping the morphology of the perovskite phase. It promotes the growth of polycrystalline grains up to several hundred nanometers, which improves the optoelectronic properties of the perovskite. This approach can also be applied for industrial-scale production and the creation of modular devices.

5. Thermal stress tests conducted under high vacuum conditions confirmed that interface engineering plays a crucial role in the stability of perovskite solar cells. An ultra-stable inverted architecture with a double-layered AZO/ SnO_x electron extraction layer (EEL) was developed. In this structure, the 20 nm thick ALD (atomic layer deposition) grown SnO_x layer acts as a dense barrier, preventing moisture ingress and the escape of decomposition products such as $\text{CH}_3\text{NH}_3\text{I}$ and HI. Furthermore, this layer proved its multifunctional effectiveness by reducing degradation caused by ion migration and preventing electrode corrosion.

**РАЗОВЫЙ НАУЧНЫЙ СОВЕТ НА ОСНОВЕ НАУЧНОГО СОВЕТА
DSc.02/30.12.2019.K/FM/T.36.01 ПО ПРИСУЖДЕНИЮ УЧЕНЫХ
СТЕПЕНЕЙ ПРИ ИНСТИТУТЕ ХИМИИ И ФИЗИКИ ПОЛИМЕРОВ**

ИНСТИТУТ ХИМИИ И ФИЗИКИ ПОЛИМЕРОВ

ЖУЛЛИЕВ ЗАВКИДДИН НОРМЕНГЛИ УГЛИ

**ВЗАИМОСВЯЗЬ ОСОБЕННОСТЕЙ ФОРМИРОВАНИЯ
ПЕРОВСКИТНОГО АБСОРБЕРА С КОНВЕРСИОННЫМИ
ПОКАЗАТЕЛЯМИ СОЛНЕЧНЫХ ЯЧЕЕК НА ЕГО ОСНОВЕ**

01.04.06 – Физика полимеров

02.00.12 – Нанохимия, нанофизика и нанотехнология

**АВТОРЕФЕРАТ ДИССЕРТАЦИИ ДОКТОРА ФИЛОСОФИИ (PhD)
ПО ФИЗИКО – МАТЕМАТИЧЕСКИМ НАУКАМ**

Ташкент – 2025

Тема диссертации на соискание ученой степени доктора философии (PhD) по физико-математическим наукам зарегистрирована в Высшей аттестационной комиссии при Кабинете Министров Республики Узбекистан под номером B2025.2.PhD/FM1331.

Диссертация выполнена в Институте химии и физики полимеров.

Автореферат диссертации на трех языках (узбекский, русский, английский) (резюме)) размещен на веб-странице Научного совета (www.polchemphys.uz) и информационно-образовательном портале «ZiyoNet» (www.ziyo.net).

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**Центр развития нанотехнологий при
Национальный университет Узбекистана имени
Мирзо Улугбека**

Защита диссертации состоится «__» **январь** 2026 г. в ____ часов на заседании Научного совета DSc.02/30.12.2019.K/FM/T.36.01 при Институте химии и физики полимеров по адресу: 100128, г.Ташкент, ул. Абдулла Кадыри, 7^б. Тел. (99871) 241-85-94, факс: (99871) 241-26-61, e-mail: polymer@academy.uz.

С диссертацией можно ознакомиться в Информационно-ресурсном центре Института химии и физики полимеров за №__ (Адрес: 100128, г. Ташкент, улица Абдулла Кадыри 7^б. Тел.: (99871) 241-85-94).

Автореферат диссертации был разослан «__» **декабрь** 2025 года.

(протокол рассылки № __ от “__” **декабрь** 2025 года).

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ВВЕДЕНИЕ (аннотация диссертации доктора философии (PhD))

Целью исследования является изучение кинетики образования перовскитового абсорбера из растворов прекурсоров в зависимости от их морфологии и определение роли специальной добавки (тиомочевины) в укрупнении поликристаллов и их взаимосвязи с эффективностью и стабильностью инвертированных солнечных элементов.

Объект исследования. Исследования сосредоточены на активных слоях MAPbI_3 перовскита, полимерном полупроводнике РТАА, служащем транспортным слоем дырок, добавке тиомочевины в качестве модификатора кристаллизации (основа Льюиса) и электронно-транспортных слоях SnO_x , а также на солнечных элементах, изготовленных на основе этих компонентов.

Научная новизна исследования заключается в следующем:

впервые выявлена закономерность нарастания полииодидных комплексов с увеличением концентрации прекурсора независимо от типа растворителя при формировании перовскитового абсорбера и этот процесс количественно подтвержден измерениями ЯМР ^{207}Pb , UV-Vis, UPS и проводимости;

впервые определена роль добавки тиомочевины в процессе кристаллизации перовскита; установлено, что она активируется в основном во время термической обработки, стимулируя рост и переориентацию кристаллов в направлении $\langle 110 \rangle$, и этот эффект связан с высокой подвижностью ионов;

разработан солнечный элемент с p-i-n структурой на основе стабильного MAPbI_3 на основе двухслойного электронно-экстракционного слоя (EEL) AZO/ SnO_x , при этом установлено, что слой SnO_x действует как многофункциональный барьер, эффективно подавляющий ионную миграцию и коррозию электродов;

Внедрение результатов исследования. На основе научных результатов, полученных по теме «Взаимосвязь особенностей формирования перовскитного абсорбера с конверсионными показателями солнечных ячеек на его основе»:

путем введения специальных добавок (аддитивов), таких как тиомочевина, в активный слой и формирования плотного барьера со слоем SnO_x , выращенным поверх активного слоя, он был использован при реализации фундаментального проекта № ИЛ-5421101892 «Изучение фундаментальных основ люминесцентных свойств энергосберегающих структур на основе полупроводниковых перовскитов», выполненного в Физико-технический институт имени С.А. Азимова Академии наук Республики Узбекистан (свидетельство № 01/467 от 8 сентября 2025 г.). Установлено, что размер кристаллитов (зерен) в активном слое CsPbBr_3 увеличивается за счет введения специальных добавок, таких как тиомочевина ($\text{SC}(\text{NH}_2)_2$), которые были успешно использованы. В фоточувствительных устройствах на основе архитектуры слоя экстракции электронов SnO_x (EEL) CsPbBr_3 достигнута долговременная эксплуатационная стабильность устройств.

результаты диссертационной работы были внедрены в рамках международного проекта «Light Harvesting in Space with Perovskite Solar Cells (SpacePerCells)», финансируемого программой НАТО «Наука ради мира и безопасности» (SPS), который реализуется совместно Вуппертальским центром «Умные материалы и системы» (Вупперталь, Германия) и Институтом химии и физики полимеров (Ташкент, Узбекистан). Разработанный в диссертации двухслойный электрон-экстрагирующий слой (EEL) на основе AZO/SnO_x, примененный в архитектуре устройства ITO/PTAA/MAPbI₃/PCBM/EEL/Ag, позволил значительно повысить долгосрочную эксплуатационную стабильность и долговечность солнечных элементов. В частности, данный слой выполняет функцию эффективного пермеационного барьера (защитного барьера), блокируя миграцию подвижных ионов из слоя перовскита и предотвращая улетучивание галогенидных соединений. Данные результаты обеспечили сохранение функциональных характеристик устройств в условиях низкого давления (вакуума), характерных для космического применения. (Подтверждающий документ: Рекомендательное письмо профессора Вуппертальского университета и справка о внедрении международного проекта).

Структура диссертации. Диссертация состоит из введения, шести глав, заключения, списка литературы и приложений. Объем диссертации составляет **102** страниц.

E'LON QILINGAN ISHLAR RO'YXATI
СПИСОК ОПУБЛИКОВАННЫХ РАБОТ
LIST OF PUBLISHED WORKS

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Avtoreferat “O‘zbekiston polimerlar jurnali” tahririyatida tahrirdan o‘tkazilib,
o‘zbek, rus va ingliz tillaridagi matnlar o‘zaro muvofiqlashtirildi.



№ 10-3279

Bosishga ruxsat etildi: 27.12.2025.

Bichimi: 60x84^{1/16} «Times New Roman»
garniturada raqamli bosma usulda bosildi.

Shartli bosma tabog‘i 2,8. Adadi 100. Buyurtma: № 205

Tel: (99) 832 99 79; (77) 300 99 09

Guvohnoma reestr № 10-3279

“IMPRESS MEDIA” MChJ bosmaxonasida chop etildi.

Manzil: Toshkent sh., Yakkasaroy tumani, Qushbegi ko‘chasi, 6-uy.