## ALD Applications
## Room Grand Ballroom H-K - Session AA2-WeA

### Energy Solar

**Moderators:** Mike McSwiney, Applied Materials, Shaibal Sarkar, ITT Bombay

4:00pm **AA2-WeA-11 Atomic Layer Deposition of Highly Stable and Efficient Perovskite Solar Cells (~ 24%)**, *H. Park, S. Shin, P. Nandi, D. Pal,* ***Hyunjung Shin***, Sungkyunkwan University (SKKU), Republic of Korea **INVITED**

Power conversion efficiency (PCE) of Perovskite solar cells (PSCs) is over 25.7%. Their operational/environmental instability remains to be solved and restrict commercialization.[1] The state-of-the-art PSC is used pure a-$FAPbI_3$ and Spiro-OMeTAD in *n-i-p* structure of PSCs. A chemical-driven transition from photoactive α-$FAPbI_3$ to non-photoactive δ-$FAPbI_3$ is pointed as a significant challenge. Much lower stability of Spiro-OMeTAD is critical for the device instability. As an interlayer in between top metallic electrodes and Spiro-OMeTAD/a-$FAPbI_3$, inorganic HTLs prepared by a low-temperature ALD provide bi-functionality to stabilize the PSCs during operation. Transition metal oxide (TMO) can be a strong candidate. Most of TMO layers generally require a high processing temperature and the lack of *p*-type characteristics inhibits application to PSCs as hole-transporting interlayers. We adopt ALD to fabricate TMO layers at low temperatures (~ 50 °C) and intentionally induce oxygen deficient traps to form empty *d*-bands and further enhance hole transporting properties. We fabricated n-i-p normal structure PSCs of a-$FAPbI_3$ and Spiro-OMeTAD with ALD grown TMOs on top of Spiro-OMeTAD to enhance device stability. We also adopt ALD to form ultra-thin NiO and $SnO_2$ as charge transport layers (ETLs).[2,3] As a result, highly efficient PSCs of PCE of over 24% with TMOs are fabricated with pin-hole free hole transporting and protection bi-functional ALD layers.[2,3] The environmental stability of PSCs is over 90% initial PCE after 600 hrs, while without the interlayer started to be degraded under 80% of initial PCE just after around 200 hrs without any special encapsulation. Furthermore, this study shows the possibility that ALD TMOs can be also applicable to tandem device fabrication with p-i-n type PSCs and stable PSCs' commercialization.

[1] High Efficiency Perovskite Solar Cells, *Chem. Rev.* (2020) [2] Perovskite Solar Cells with Inorganic Electron and Hole Transporting Layers Exhibiting Long – Term (≈ 500 h) Stability at 85 °C under Continuous 1 Sun Illumination in Ambient Air, *Adv. Mater.* (2018) [3] Atomic Layer Deposition for Efficient and Stable Perovskite Solar Cells, *Chem. Comm.* (2019) [4] Cyclohexylammonium-Based 2D/3D Perovskite Heterojunction with Funnel-Like Energy Band Alignment for Efficient Solar Cells (23.91 %), *Adv. Energy Mater.*(2021) [5]Amorphous $TiO_2$ Coatings Stabilize Perovskite Solar Cells, *ACS Energy Lett*(2021)[6] Hole Transporting Vanadium-Containing Oxide ($V_2O_{5-x}$) Interlayers Enhance Stability of a-$FAPbI_3$-Based Perovskite Solar Cells (~ 23%), *ACS Appl. Mater. & Interfaces,* (2022)

4:30pm **AA2-WeA-13 ALD of Niobium Oxide ($Nb_2O_5$) and Niobium-doped Titanium Oxide (Nb:$TiO_2$) for Solar Cell Applications**, *T. VINCENT,* IPVF, France*; D. COUTANCIER,* CNRS, France*; P. Dally, M. AL-KATRIB, F. DONSANTI,* IPVF, France*; A. YAICHE,* EDF, France*; K. MEDJOUBI, M. PROVOST,* IPVF, France*; J. ROUSSET,* EDF, France*; M. BOUTTEMY,* ILV, France*;* ***Nathanaelle SCHNEIDER***, CNRS, France

Atomic Layer Deposition (ALD) is increasingly contributing to the energy field and more specifically to the engineering of solar cells. Its conformity enables deposition on nanostructured substrates and its low growth temperature allows the deposition on temperature-sensitive substrates such as perovskite. Niobium oxide, $Nb_2O_5$, is a wide bandgap semiconductor that has been grown by different methods and has recently been used in solar cells. Its optical and electrical properties depend strongly of the technique used for its growth, opening access to a wide range of application, such as electron transport layer (ETL)or passivation layer [1,2]. It is also used for the doping of titanium oxide ($TiO_2$), a well-known ETL, to reach a better stability of the complete solar cell.

In this study, the growth of niobium-doped titanium oxide ($TiO_2$:Nb) thin films by atomic layer deposition (ALD) is reported. Films were obtained at 200°C from titanium (IV) i-propoxide (TTIP), (t-butylimido)tris(diethylamido)niobium(V) (TBTDEN), and water by introducing $Nb_2O_5$ growth cycle in a $TiO_2$ matrix. Process parameters such as the order of precursor introduction and the cycle ratio were optimized. The growth mechanisms and the effective Nb incorporation were investigated by in situ quartz crystal microbalance (QCM) and X-ray photoelectron spectroscopy (XPS). The as-deposited films were analyzed for their surface morphology, elemental stoichiometry, optoelectronic properties, and crystallinity using a variety of characterization techniques. Such as-deposited films are amorphous and a fine control of the Nb amount with the supercycle parameters along with a continuous evolution of their optical properties from the ones of $TiO_2$ to $Nb_2O_5$ bare oxides are observed. To allow a successful implementation in solar devices, a comprehensive annealing study under several temperatures and atmospheres was conducted and revealed an evolution of the optical bandgap after crystallization in the anatase phase. Ultimately, the incorporation of these 15 nm-thick films in mesoscopic perovskite solar cells (PSCs) as ETL shows an improvement of the cell performances and of their stability with increasing Nb amount, reaching power conversion efficiency (PCE) up to 19.8%.

[1] Subbiah, et al (2019). *Energy Technology, 8*(4), 1900878. https://doi.org/10.1002/ente.201900878

[2] Macco et al, (2018). *Solar Energy Materials and Solar Cells, 184*, 98-104. https://doi.org/j.solmat.2018.04.037

4:45pm **AA2-WeA-14 Closing Remarks**,

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