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Lead-free metal halide perovskites

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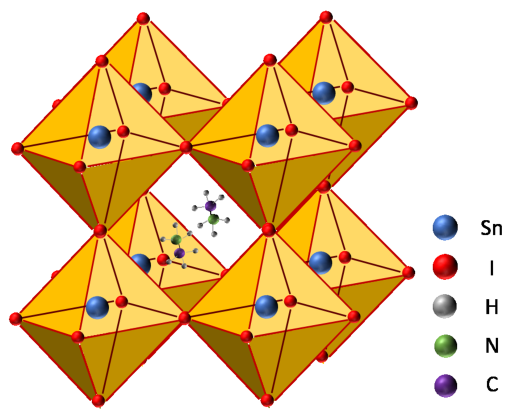
IMP

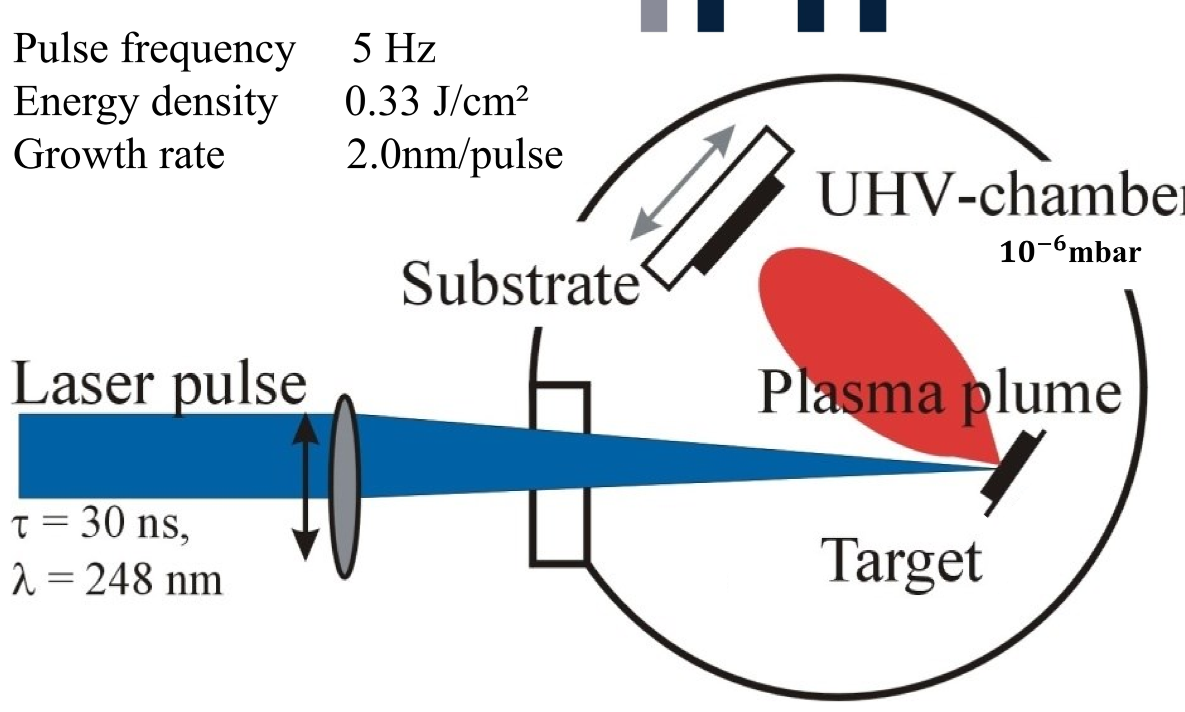
Materials system

Online guided tour through the poster:

Lead-free hybrid organic-inorganic perovskite solar cells represent an economically and environmentally viable alternative to conventional photovoltaic modules. Although, there is a mayor drawback of photo- and humidity-induced degradation attributed to ion migration and decomposition of the lattice structure in the absorber layer.

We want to fabricate perovskite thin films that contain iodine in interstitial positions since their occupation by lattice iodine species is assumed to be the governing degradation channel [1]. The deposition of such supersaturated phases is enabled due to the strong non-equilibrium conditions during PLD and was firstly demonstrated in 2015 [2]. The optimization of the homogeneity is key for improving energy conversion since many/small grain boundaries/sizes limit the carrier diffusion lengths [3] and hence shorten their lifetime, because they act as pinning centers and foster recombination of differently charges species [4].

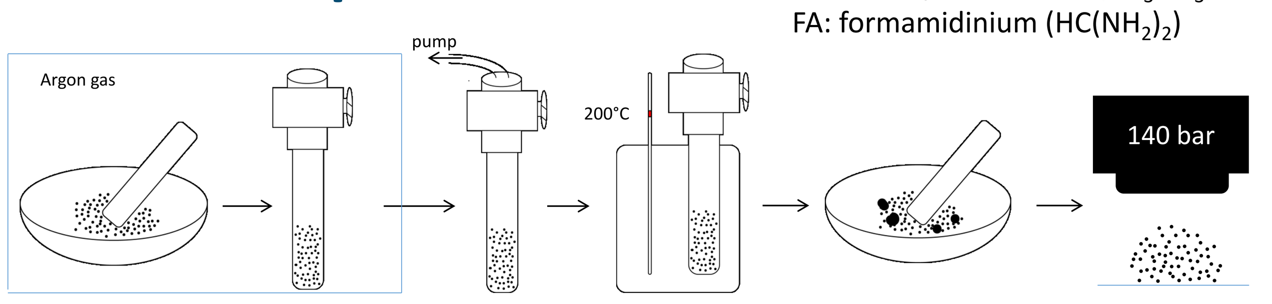




Fabrication and characterization of targets

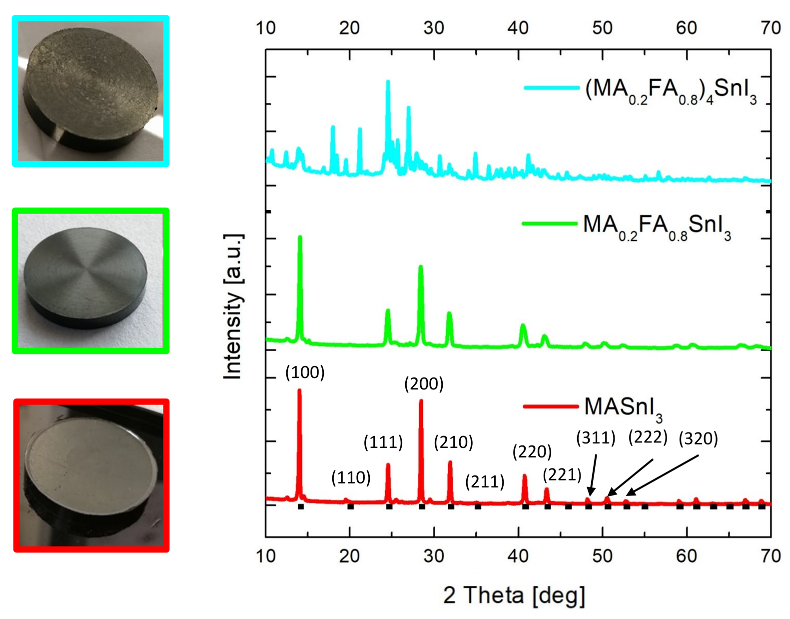
Process sequence

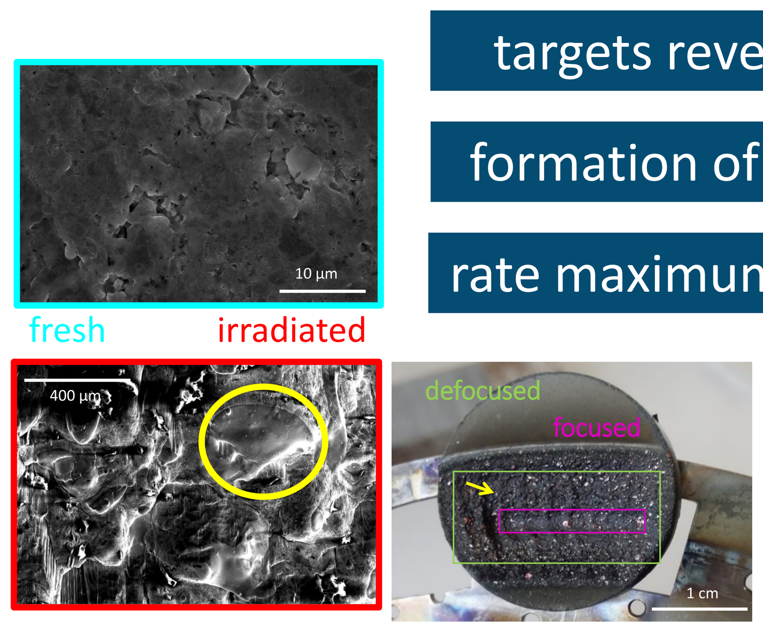
MA: methylammonium (CH_3NH_3)
FA: formamidinium ($HC(NH_2)_2$)



$$CH_3NH_3I + SnI_2 \xrightarrow{200^\circ C} CH_3NH_3SnI_3$$

targets manufactured by solid state reaction of powders

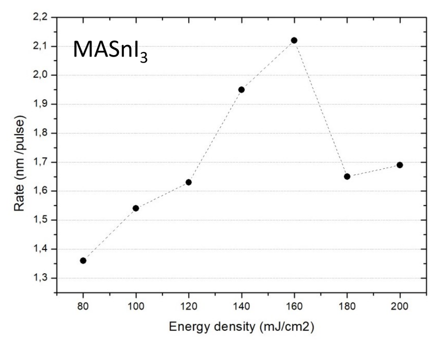




targets reveal perovskite structure

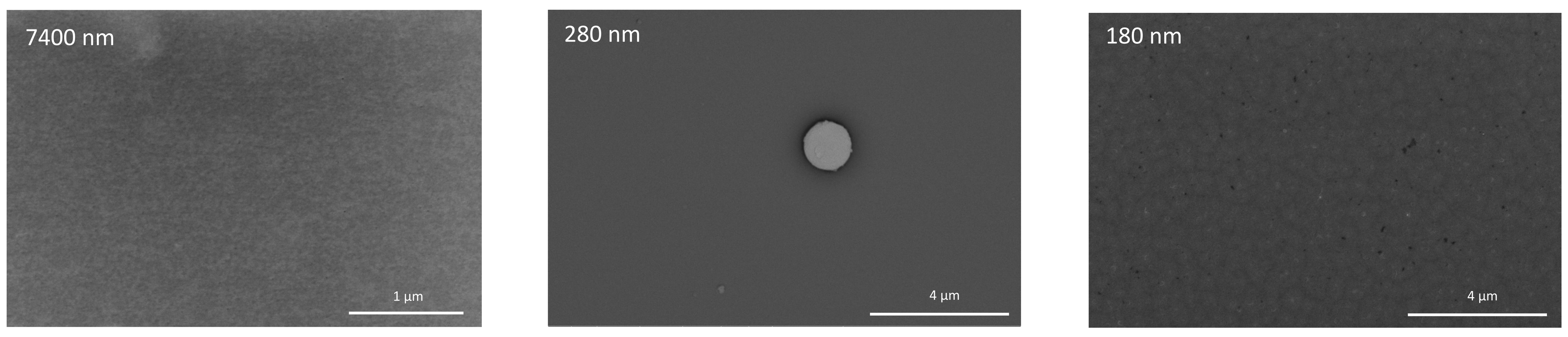
formation of $SnI_{2-\delta}$ during irradiation

rate maximum due to decompostition

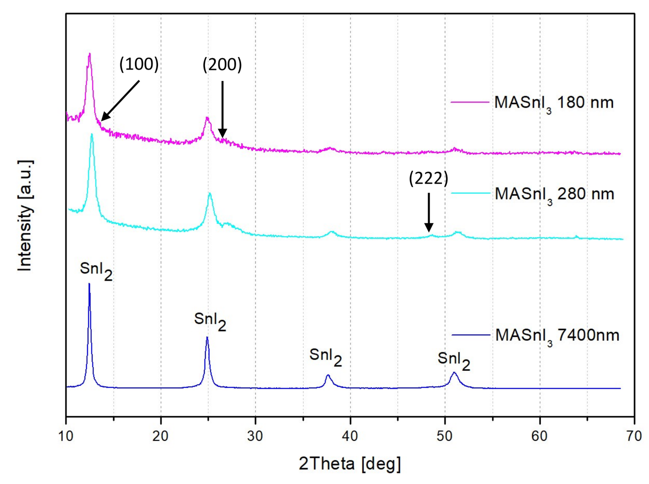


Structural and morphological analysis of thin films

$MASnI_3$



uniform and smooth | compact layer | pores and voids



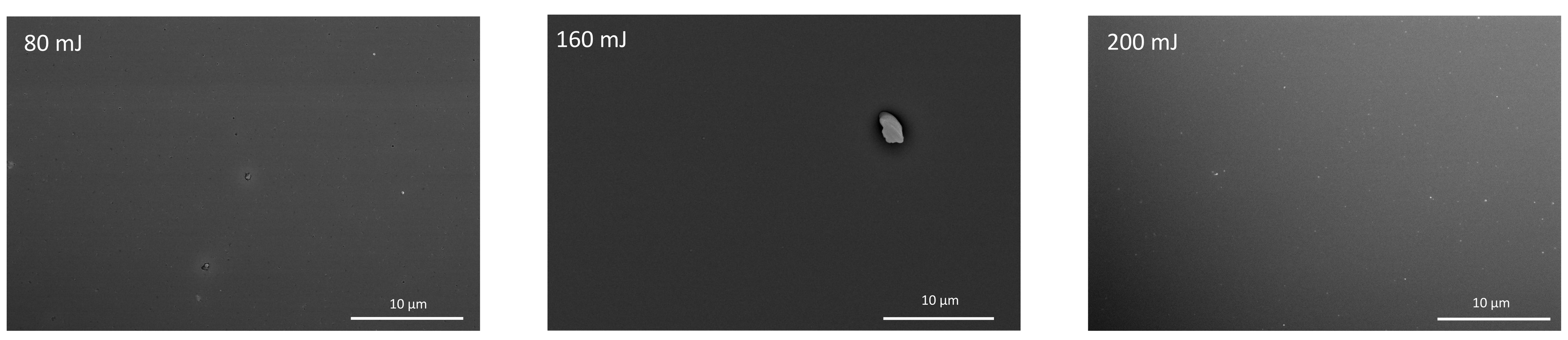
wide beam leads to higher rate

average droplet diameter: 230 nm

SnI_2 dominates crystalline structure

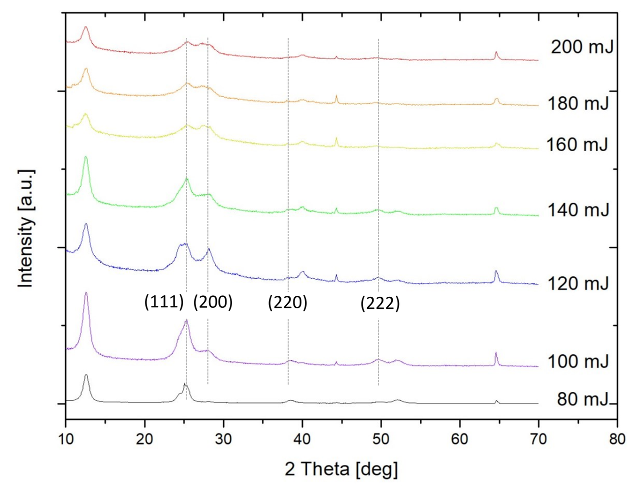
MA instable ⇨ doping with FA

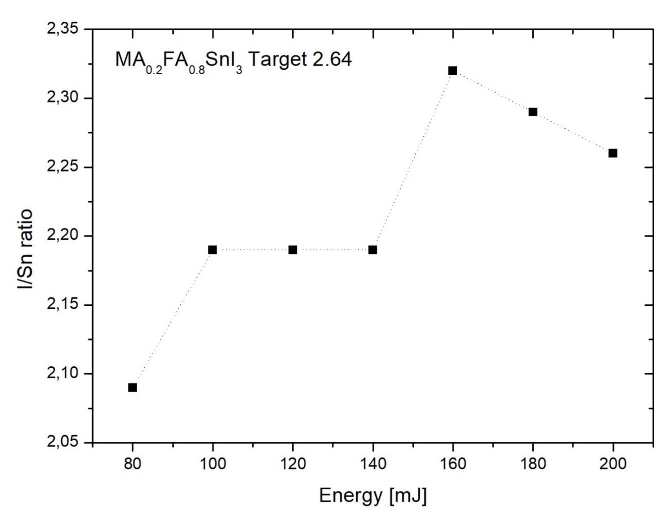
$MA_{0.2}FA_{0.8}SnI_3$



least content of SnI_2 at 160 mJ

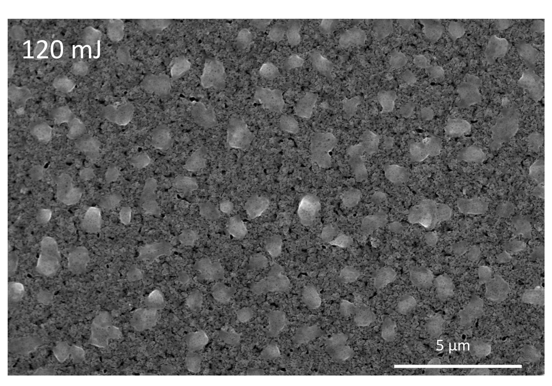
I/Sn ratio of target and film incorrect





increased temperatures up to 120°C lead to loss of organic component

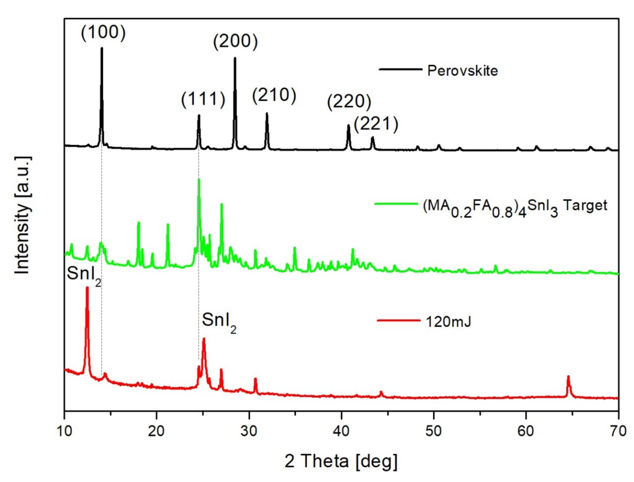
$(MA_{0.2}FA_{0.8})_4SnI_3$



reduced energy density: I/Sn ratio in film 2.42

residuals of non-perovskite target-structures

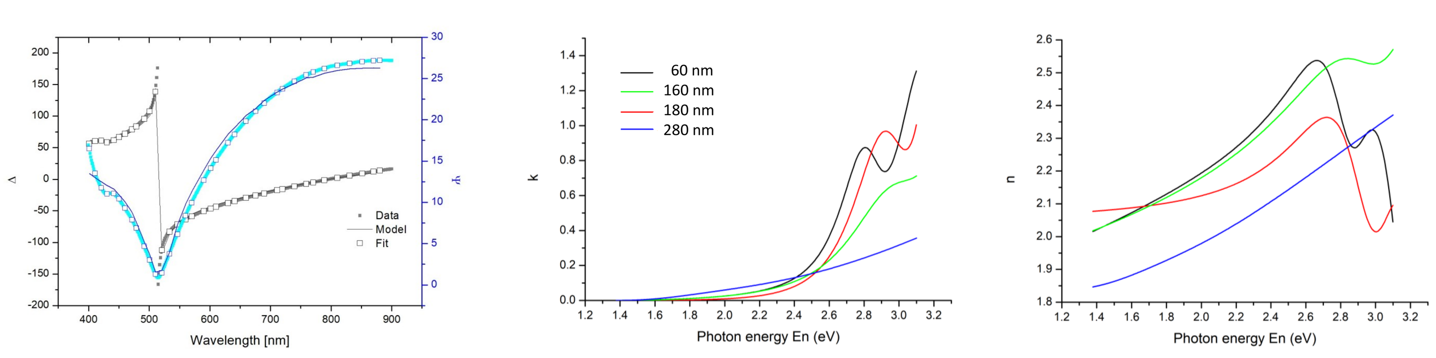
large crystallites mainly of organic-rich phase



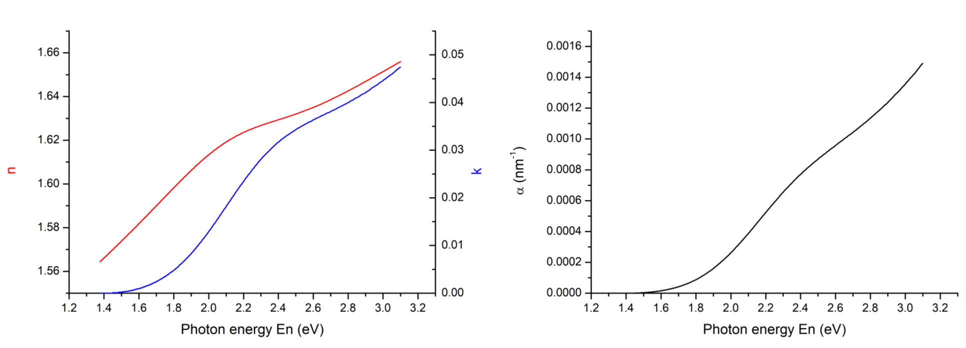
Outlook:
- □ studies on phase transitions via TGA and DSC and *in-situ* XRD
- □ further increase of organic component
- □ annealing at low temperatures
- □ detailed structural analysis

Optical properties examined by spectroscopic ellipsometry

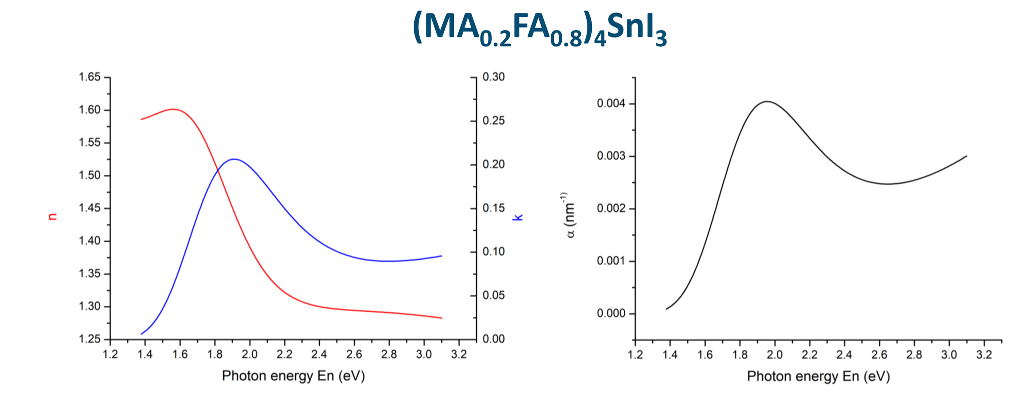
$MASnI_3$



$MA_{0.2}FA_{0.8}SnI_3$



$(MA_{0.2}FA_{0.8})_4SnI_3$



Forouhi-Bloomer model

properties change with film thickness

$MASnI_3$	$MASnI_3$	$MA_{0.2}FA_{0.8}SnI_3$	$(MA_{0.2}FA_{0.8})_4SnI_3$	$(MA_{0.25}FA_{0.75})_4SnI_3$
1.30-1.37 eV [5]	1.3 eV	1.4 eV	1.48 eV	1.4 eV [6]

Outlook: structure-property relations

[1] G. Y. Kim, A. Senocrate, T.-Y. Yang, G. Gregori, M. Grätzel, and J. Maier, Nature materials, vol. 17, no. 5, p. 445 (2018)
[2] U. Bansode, R. Naphade, O. Game, S. Agarkar, and S. Ogale, The Journal of Physical Chemistry C, vol. 119, no. 17, pp. 9177–9185 (2015)
[3] T. Matsushima, T. Fujihara, C. Qin, S. Terakawa, Y. Esaki, S. Hwang, A. S. Sandanayaka, W. J. Potscavage, and C. Adachi, Journal of Materials Chemistry A, vol. 3, no. 34, pp. 17780–17787 (2015)
[4] P. Scajev, R. Aleksiejunas, S. Miasojedovas, S. Nargelas, M. Inoue, C. Qin, T. Matsushima, C. Adachi, and S. Jursenas, The Journal of Physical Chemistry C, vol. 121, no. 39, pp. 21600–21609 (2017)
[5] L. Jiang, T. Wu, L. Sun, Y.-J. Li, A.-L. Li, R.-F. Lu, K. Zou and W.-Q. Deng J. Phys. Chem. C 121, 24359-24364 (2017)
[6] N. Ito, M. A. Kamarudin, D. Hirotani, Y. Zhang, Q. Shen, Y. Ogomi, S. Iikubo, T. Minemoto, K. Yoshino and S. Hayase J. Phys. Chem. Lett. 9, 1682–1688 (2018)