Chapter 5
Conclusions

5.1 Synthesis and characterization of well-aligned TiO_2 NRs

Effect of the TiO_2 seed layers on the growth of TiO_2 NRs	• SLs with a lower surface roughness contribute to orderly grown tetragonal rutile NRs in vertical align. • The oriented NRs were obtained significantly which could be suit to apply as ETL in perovskite solar cell for improvement of electron transport. SLs can also improve TiO_2 NRs crystallinity providing TiO_2 with high density.
Effect of calcination treatment at high temperature on morphology and size of TiO_2 NRs	• The calcination could improve crystallinity of NRs by promoting oxygenation in incomplete Ti-complexes to form complete TiO_2.
Effect of precursor concentrations	• An increase of the TBO concentration favoured a simultaneous increase in average diameter and length of TiO_2 NRs • If TBO concentration is not sufficient (0.1 %TBO) to begin nucleation of NRs, the NRs could not be successfully formed. • The plane and its d-spacing effect on electrons in E_g because (002) plane with small d-spacing requires more energy to break the bound and to create free electrons, leading to higher E_g in 1.0 % TBO NRs than that in 0.7 % TBO NRs which consist of high d-spacing (101) plane.

	• Hence, geometry inside NRs effect on optical properties of NRs. • Regarding to orientation of NRs and optical properties, 0.7 % TBO NRs is the good candidate because it provides high transparent compared to 1.0 % TBO NRs and has high vertical alignment relative to 0.3 % and 0.5 % TBO NRs. • 0.7 % TBO NRs had well space between NRs which could promote penetration of Perovskite layer. Owing to the adequate NRs size and proper inter-rod spacing are significant to promote electron transfer. While, too short NRs do not offer a sufficient charge separation because their lengths are too short. Too long and densely packed NRs result in poor penetration of Perovskite. This contributes to electron-hole recombination because electron diffusion length is shorter than length of NRs [6].
Hydrothermal synthesis of TiO_2 NRs at different hydrothermal times	• Dimensions of NRs increase with the extensive times • SEM showed that NRs incredibly grew in length from 1 h to 1. 5 h indicating that olation, the formation of long chains of highly protonated Ti-complexes, which occurred the most during 1 h to 1. 5 h and slowed down at 2 h. Oxolation, the construction of lateral arrangement of Ti-complexes , could assist olation to continue which means diameter of NRs need to expand with length. On account of oxolation taking place less than olation, diameters of NRs were smaller than the length.

	• TEM results could support XRD results and describe growth mechanism during hydrothermal reaction • SEAD illustrate that 0.7 % TBO NRs and 1.0 % TBO NRs have single crystalline structure growth along [0 0 1] while (002) plane is the dominant facet • (101) growing parallel to the length of NRs is a result from olation (002) while (101) align in lateral is a result of oxolation. • The obtained single-crystal TiO_2 NRs could play an important role in solar cell application, because NRs offer fast electron pathway via the length with less grain boundary. In addition, fewer defect trap presents in single crystal NRs compared to poor crystalline leading to lower recombination [44].

5.2 Suggestions and future perspectives

5.2.1 Suggestions

1) In this work, it was overlooked during hydrothermal process because the hydrothermal synthesis occurs in a close system and high pressure. Then the autoclaves should be closed hermetically.
2) Exceed of precursor concentration could provide non homogeneous NR structure and clusters of TiO_2 NRs on the primitive NRs surface. Moreover, clusters of TiO_2 NRs consist of poor vertical oriented NRs that grew in various directions which is not appropriate to apply in Perovskite solar cells (PSCs). For Perovskite solar cell application, optimization of the precursor concentration might be of interest.

5.2.1 Future perspectives

1) It would be interesting point for future study in terms of temperature and time of calcination which can control development of NRs.

2) The round of spin coating for TiO_2 thin film preparation is also important for the diameter and density of NRs.
3) 0.7% TBO NRs should be applied as ETL in Perovskite solar cells (PSCs) in aspect of enhancement of photo conversion efficiency. Because 0.7% TBO NRs possess higher vertical arrangement relative to 0.3%- and 0.5% TBO NRs. Since the present of vacancies on substrate surface of 0.3%- and 0.5% TBO NRs and the poor alignment NRs could lead to electron transfer disorderly. Comparing to 1.0% TBO NRs, 0.7% TBO NRs are more transparent allowing more penetration of visible light to Perovskite layer which is likely to promote enhancement of light harvesting efficiency in PSCs. Therefore, 0.7% TBO NRs could be the good candidate to employ in PSCs
4) Surface of 0.3%- and 0.5% TBO NRs and the poor alignment NRs lead to electron transfer disorderly. Comparing to 1.0% TBO NRs, 0.7% TBO NRs are more transparent allowing more penetration of visible light to Perovskite layer which is likely to promote enhancement of light harvesting efficiency in PSCs. Therefore, 0.7% TBO NRs is the good candidate to employ in PSCs.