

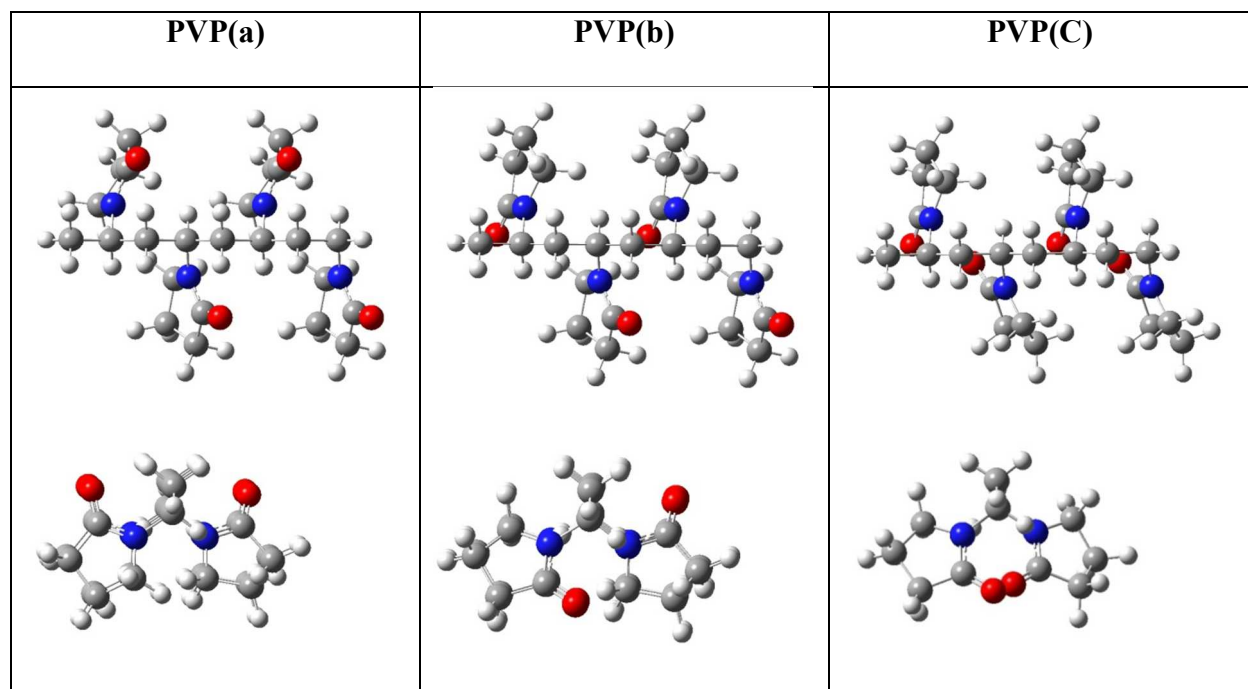
# Supporting information

## Single Crystalline-like TiO<sub>2</sub> Nanotube Fabrication with Dominant (001) Facets using Poly(vinylpyrrolidone)

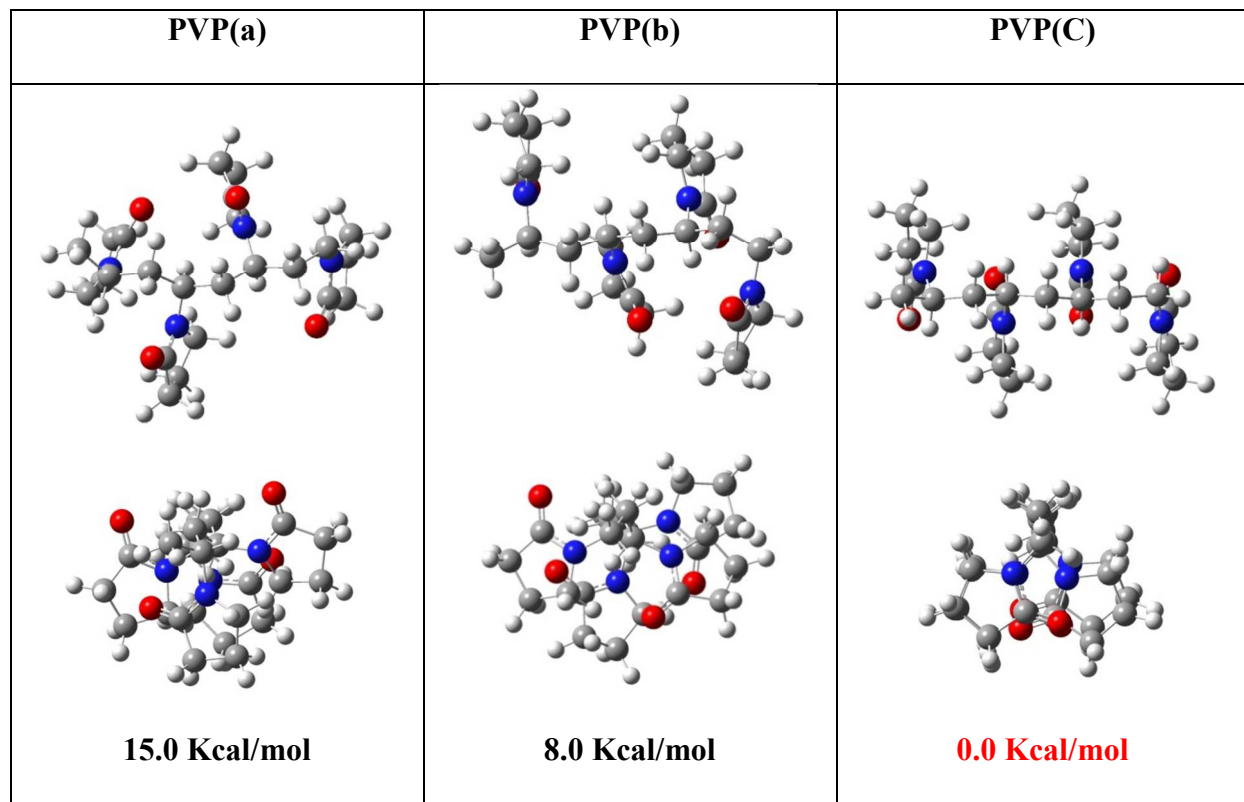
*Mi-Hee Jung<sup>\*†</sup>, Kyoung Chul Ko<sup>‡</sup>, Jin Yong Lee<sup>‡</sup>*

<sup>†</sup> Solar Cell Technology Research Section, IT Components and Materials Industry Technology  
Research Department, IT Materials and Components Laboratory, Electronics and  
Telecommunications Research Institute (ETRI), 218 Gajeong-no, Yuseong-gu, Daejeon 305-700,  
Republic of Korea. Fax: +82 (42) 860-6495; Tel: +82 (42) 860-5201; E-mail: [mhjung@etri.re.kr](mailto:mhjung@etri.re.kr).

<sup>‡</sup> Department of Chemistry, Sungkyunkwan University, Suwon, 440-746, Korea.



**Figure S1.** Three initial structures for designed PVP ( $m=4$ ) conformers. Atoms are represented as blue (N), red (O), grey (C) and white (H).



**Figure S2.** Optimized structures and relative energies (in Kcal/mol) for designed PVP ( $m=4$ ) conformers with M06/6-31G(d) level at Gaussian 09. Atoms are represented as blue (N), red (O), grey (C) and white (H).

## *References:*

23 Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J. A., Jr.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Keith, T.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, M. J.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, O.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. *Gaussian 09, Revision B.01*; Gaussian, Inc.: Wallingford, CT, **2010**.