

# Supporting Information

for

## **Functionalized TiO<sub>2</sub> nanoparticles by single-step hydrothermal synthesis: the role of the silane coupling agents**

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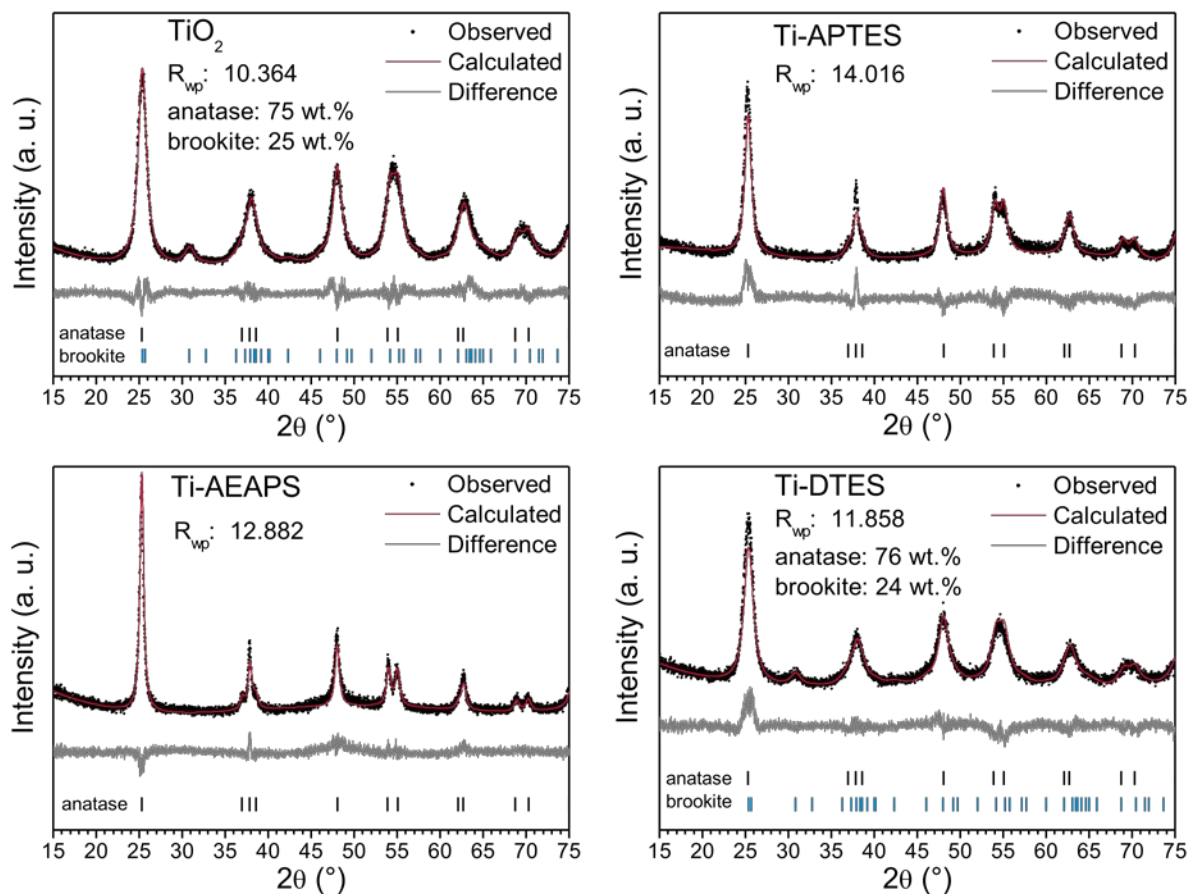
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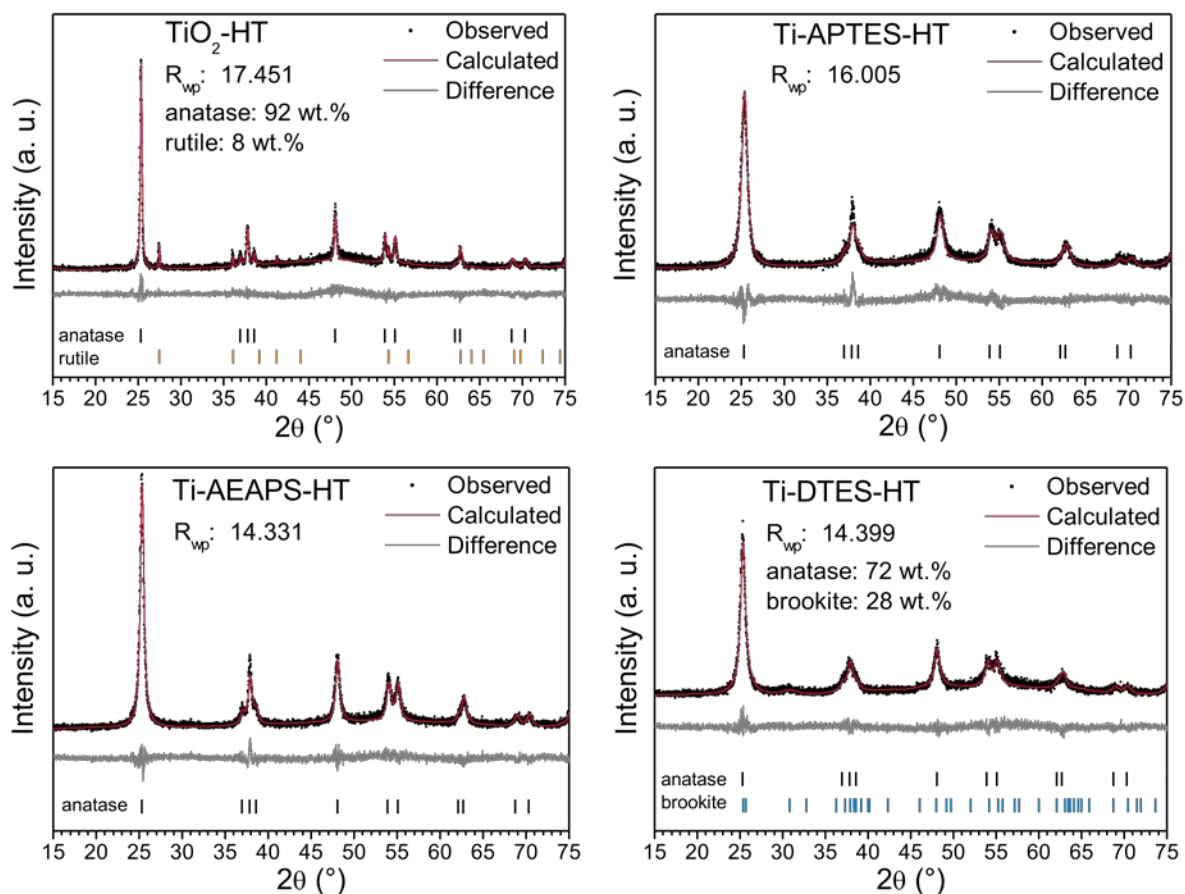
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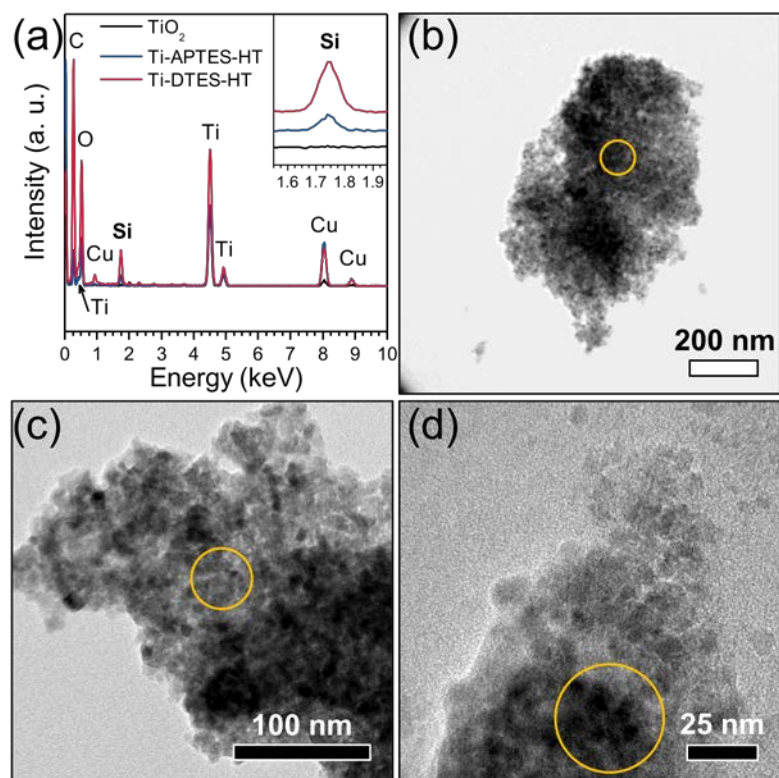
### **Additional experimental data**



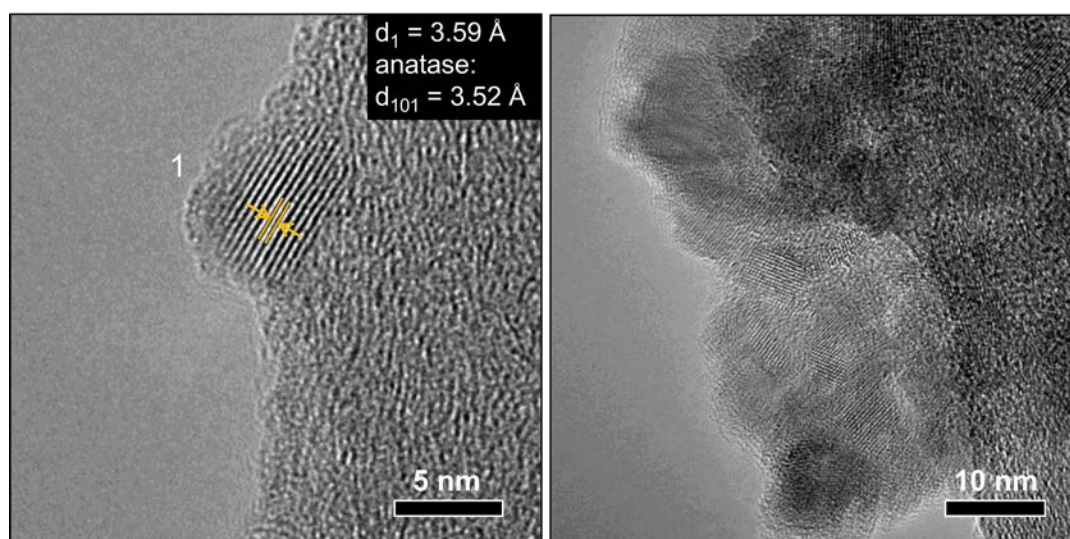
**Figure S1:** Rietveld refinements of TiO<sub>2</sub> and in situ surface-functionalized TiO<sub>2</sub> nanoparticles diffractograms (bars show diffraction lines of anatase from ICDD card #00-021-1272 and brookite from ICDD card #00-029-1360).



**Figure S2:** Rietveld refinements of heat treated TiO<sub>2</sub> and in situ surface-functionalized TiO<sub>2</sub> nanoparticles diffractograms (bars show diffraction lines of anatase from ICDD card #00-021-1272, brookite from ICDD card #00-029-1360, and rutile from ICDD card #00-021-1276).



**Figure S3:** (a) EDS spectra from samples area (yellow circles) shown on TEM images of (b)  $\text{TiO}_2$ , (c) Ti-APTES-HT, and (d) Ti-DTES-HT, respectively.



**Figure S4:** HR-TEM images of Ti-APTES-HT.

**Table S1:** Assignments of characteristic IR-bands of TiO<sub>2</sub> and *in situ* surface functionalized TiO<sub>2</sub> nanoparticles.

wave number (cm <sup>-1</sup> )	assignment	sample	references
<900	Ti–O–Ti	all	[1-4]
910	Ti–O–Si	all functionalized samples	[1-6]
1020 and 1120	Si–O–Si	all functionalized samples	[1-8]
1220	Si–CH <sub>2</sub> R	all functionalized samples	[3,5,8]
1260	Si–CH <sub>3</sub>	Ti-AEAPS	[3,5,9]
1380	CH <sub>3</sub> (deformation)	Ti-DTES	[3]
1460	CH <sub>2</sub> (deformation)	all functionalized samples	[3,8,10]
1530 and 3200–3500	N–H	Ti-APTES, Ti-AEAPS	[1,3,8,10]
1640 and 2500–3600	adsorbed H <sub>2</sub> O and OH groups	all	[1,3,7,8]
2850 and 2920	CH <sub>2</sub> (stretching)	all functionalized samples	[1-3,8,11]
2870 and 2960	CH <sub>3</sub> (stretching)	Ti-DTES	[3,11]

## References

- [1] Zhao, J.; Milanova, M.; Warmoeskerken, M. M. C. G.; Dutschk, V. *Colloids Surf., A* **2012**, *413*, 273–279. doi:10.1016/j.colsurfa.2011.11.033
- [2] Wang, C.; Mao, H.; Wang, C.; Fu, S. *Ind. Eng. Chem. Res.* **2011**, *50*, 11930–11934. doi:10.1021/ie200887x
- [3] Socrates, G. *Infrared and Raman characteristic group frequencies: Tables and charts*; John Wiley & Sons: Chichester, UK, 2001.
- [4] Koziej, D.; Fischer, F.; Kränzlin, N.; Caseri, W. R.; Niederberger, M. *ACS Appl. Mater. Interfaces* **2009**, *1*, 1097–1104. doi:10.1021/am9000584
- [5] Matinlinna, J. P.; Laajalehto, K.; Lassila, L. V. J.; Yli-Urpo, A.; Vallittu, P. K. FT-IR and XPS surface characterization of allyltrimethoxysilane and 3-

- methacryloxypropyltrimethoxysilane mixture adsorbed onto titanium substrate. In *Silanes and other coupling agents*; K. L. Mittal, Ed.; CRC Press: Boca Raton, FL, USA, 2004; Vol. 3, pp 21–37. doi:10.1201/b12184-5
- [6] Milanesi, F.; Cappelletti, G.; Annunziata, R.; Bianchi, C. L.; Meroni, D.; Ardizzone, S. *J. Phys. Chem. C* **2010**, *114*, 8287–8293. doi:10.1021/jp1014669
- [7] Chen, Q.; Yakovlev, N. L. *Appl. Surf. Sci.* **2010**, *257*, 1395–1400. doi:10.1016/j.apsusc.2010.08.036
- [8] Plodinec, M.; Gajović, A.; Iveković, D.; Tomašić, N.; Zimmermann, B.; Macan, J.; Haramina, T.; Su, D. S.; Willinger, M. *Nanotechnology* **2014**, *25*, 435601. doi:10.1088/0957-4484/25/43/435601
- [9] Czarnobaj, K. *Polym. Bull.* **2011**, *66*, 223–237. doi:10.1007/s00289-010-0332-8
- [10] Iijima, M.; Kobayakawa, M.; Kamiya, H. *J. Colloid Interface Sci.* **2009**, *337*, 61–65. doi:10.1016/j.jcis.2009.05.007
- [11] Porter, M. D.; Bright, T. B.; Allara, D. L.; Chidsey, C. E. D. *J. Am. Chem. Soc.* **1987**, *109*, 3559–3568. doi:10.1021/ja00246a011