

Supporting Information

Silicon nanosheets and their self-assembled regular stacking structure

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XANES spectra. XANES spectroscopy provides information on local atomic and electronic structures around an absorbing atom. The TEY mode is effectively used for monitoring the surface region. On the other hand, FY mode has detection sensitivity to a depth of approximately 100 nm. The Si-*K* edge absorption spectrum of C10-Si_n obtained using the FY mode in a He atmosphere is shown in Figure S1, with those of quartz and β-Si₃N₄ included for comparison. The large peak around 1844 eV for C10-Si_n is very close to that observed in β-Si₃N₄. The peak position is different from those of crystalline silicon (near 1840 eV), siloxene (near 1846 eV), or layered polysilane (near 1840 eV)^{S1}, which suggests that C10-Si_n contains Si-N-Si linkages and no Si-O linkages. The spectra shown here are the same as those in Figure 3. C10-Si_n forms highly stacked structure on the HOPG plate, as revealed by XRD, and the chemical structure near the surface region is not different to that in the inner region. However, a small peak near 1846 eV appeared in C10-Si_n after long term exposure to air. The chemical stability against oxygen seems to be weaker than the amine-modified Si(100) surface of bulk, porous silicon or silicon nanoparticles^{S2, S3}.

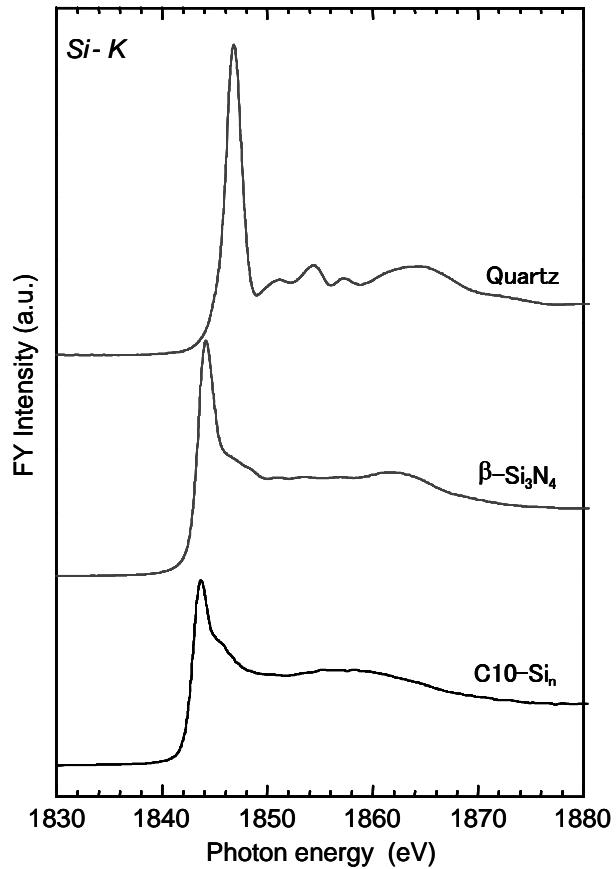


Figure S1. Comparison of XANES spectra of C10-Si_n with quartz and β-Si₃N₄ obtained using FY mode in a He atmosphere. A large peak around 1844 eV was detected for both C10-Si_n and β-Si₃N₄, which suggests that C10-Si_n contains Si-N-Si linkages.

References

- S1. Dahn, J. R.; Way, B. M.; Fuller, E.; Tse, J. S. *Phys. Rev B.* 1993, **48**, 17872-17877.
- S2. Bergerson, W. F.; Mulder, J. A.; Hsung, R. P.; Zhu, X.-Y. *J. Am. Chem. Soc.* 1999, **121**, 454-455).
- S3. Rogozhina, E.; Belomoin, G.; Smith, A.; Abuhassan, L.; Barry, N.; Akcakir, O.; Braun, P. V.; Nayfeh, M. H.; *Appl. Phys. Lett.* 2001, **78**, 3711-3713.

Complete reference 35

Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, J. A. Jr.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; 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.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; J. A. Pople, J. A. *Gaussian 03*, Revision E.01, Gaussian Inc., Wallingford CT, 2004.