



Supporting Information

for

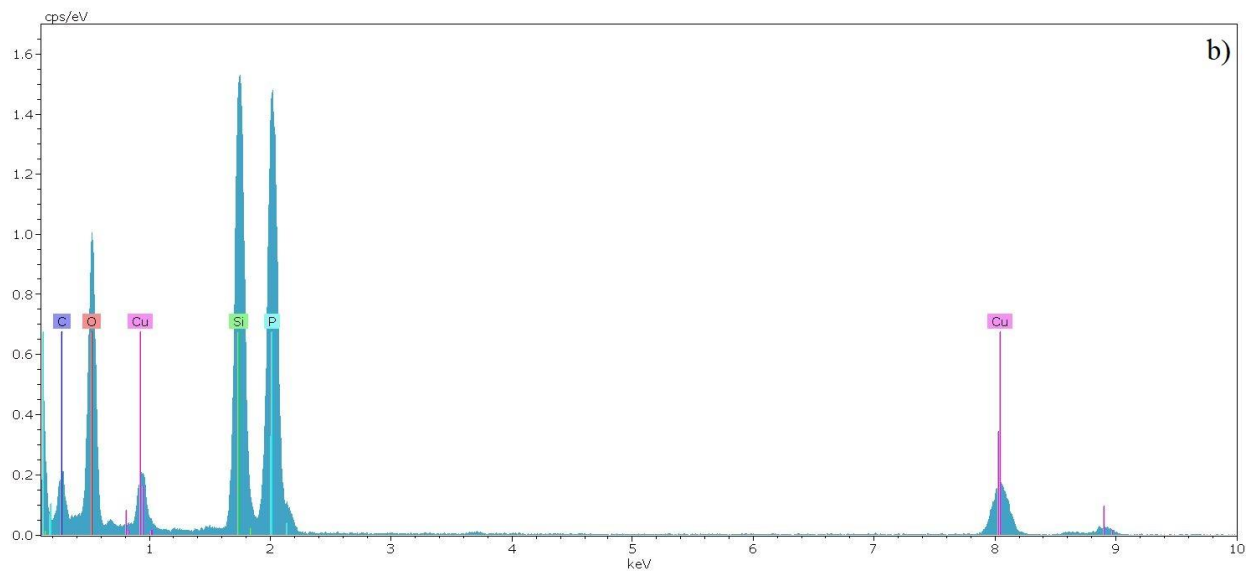
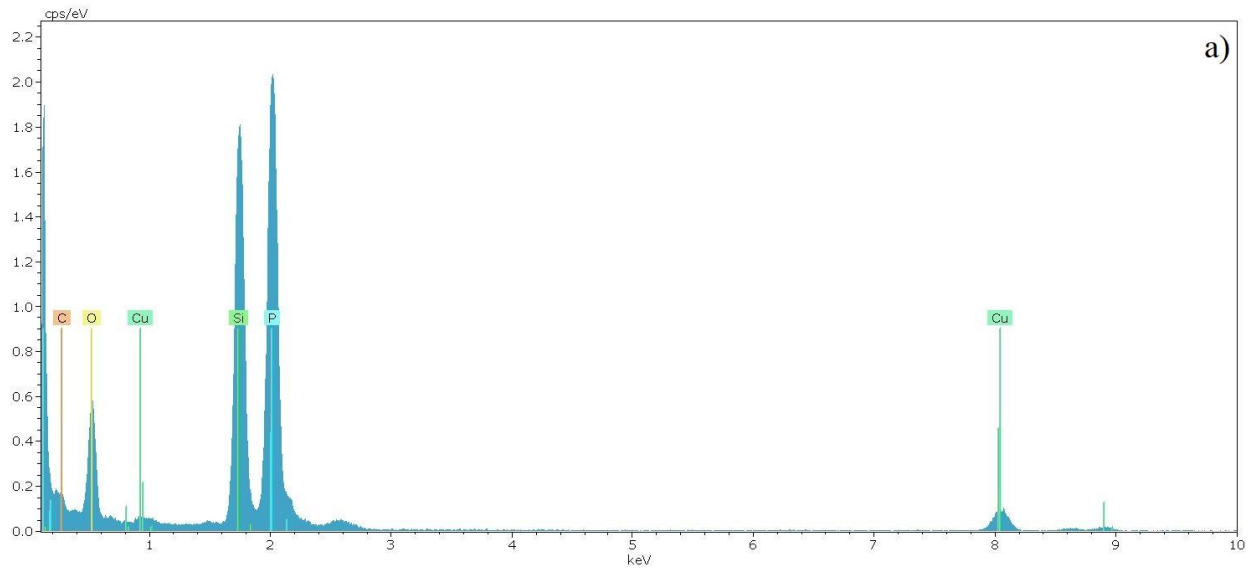
Isolation of cubic Si_3P_4 in the form of nanocrystals

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Additional experimental data

Selected temperature for doping of Si NPs with phosphorus and the calculation of the diffusion constant resulted from the equation $D = D_0 e^{\frac{-Q}{RT}}$, where $D_0=20 \text{ cm}^2/\text{sec}$, $Q=364 \text{ kJ/mol}$, $T=670^\circ\text{C}$ [1].



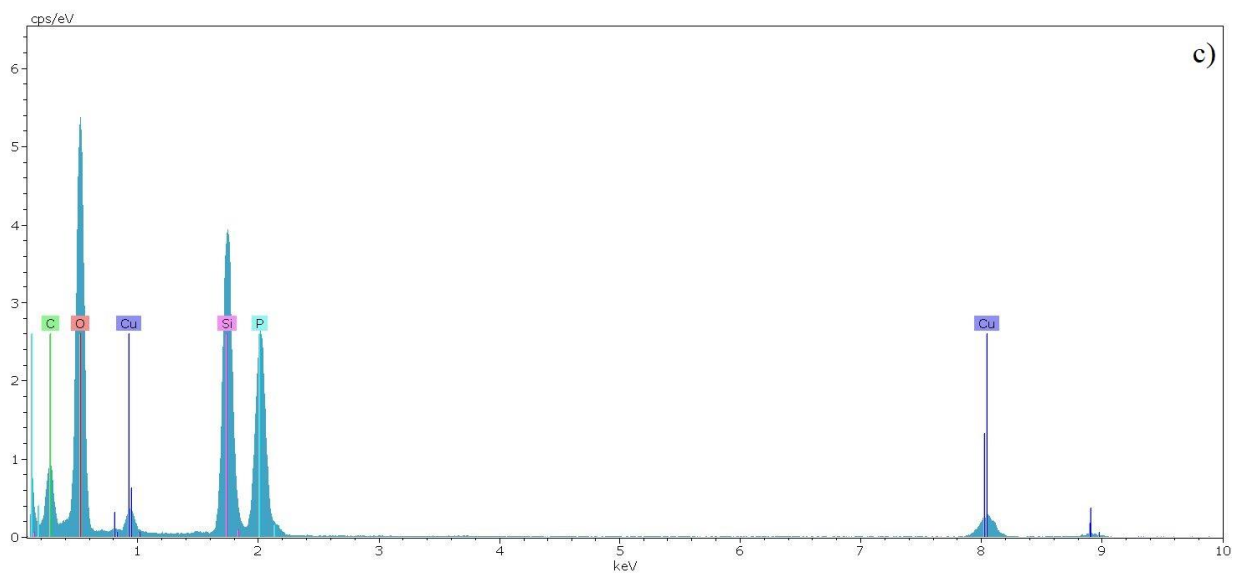


Figure S1: EDX spectra of (a),(b) – SP550, (c) – SP670.

Table S1: The correlation of bands and wavenumbers for Si NPs, hydrogenated Si NPs and SP400, SP670 and SP900 samples.

| Assignment | Wavenumber, cm ⁻¹ | | | | | |
|-------------------------------------|------------------------------|--------|---------------------|--------------------|-------|-------|
| | Reference data | Sample | | | | |
| | | Si NPs | Hydrogenated Si NPs | SP400 | SP670 | SP900 |
| O-H stretching | 3700-3200 [2] | 3420 | 3509 3450 | - | 3450 | 3329 |
| =C-H stretching | 3100-3000 [2] | - | - | 3073 | - | - |
| Methyl asymmetric C-H stretching | 2960 [3] | 2960 | 2957 | 2956 | 2960 | 2956 |
| Methylene asymmetric C-H stretching | 2930 [2] | 2925 | 2924 | 2925 | 2926 | 2921 |
| Methylene symmetric C-H stretching | 2850 [2] | 2854 | 2855 | 2853 | 2857 | 2853 |
| (O ₃)Si-H stretching | 2250 [4] | 2267 | - | - | - | 2266 |
| (Si ₃)Si-H stretching | 2100 [4] | 2105 | 2107 | - | - | - |
| Overtone HRC=CH ₂ | 1850-1800 [3] | | | 1821 | | |
| C=O stretching | 1730 [2] | 1728 | 1711 | 1743-1730- 1718 | 1714 | 1720 |
| H ₂ O deformation | 1640 [5] | 1623 | 1631 | - | 1646 | 1641 |
| C=C stretching | 1680-1600 [2] | - | - | 1642 | - | - |
| Methylene scissoring | 1465 [2] | 1465 | 1466 | 1466 | 1469 | 1465 |
| Methyl symmetrical C-H bending | 1380 [2] | - | - | 1378 | - | - |

| | | | | | | |
|------------------------------------|-----------------------|--------------|--------------|--------------|--------------|--------------|
| Methylene twisting | 1300 [2] | - | - | 1302 | - | - |
| Si-O-Si stretching | 1200-1000 [2], [6] | 1208 1069 | 1167 1072 | 1186 1098 | 1205 1090 | 1183 1073 |
| C-H deformation non-planar (vinyl) | 995-985 [3] | - | - | 992 | - | - |
| C-H deformation non-planar (vinyl) | 915-905 [3] | - | - | 911 | - | - |
| H-Si-O ₃ deformation | 880 [6] | 880 | - | - | - | 874 |
| H-Si-O ₂ deformation | 850 [6] | - | 863 | - | - | - |
| Si-O-Si symmetrical stretching | 810 [7] | 804 | 814 | 806 | 801 | 806 |
| Methylene rocking | 720 [2] | - | 720 | 721 | - | - |
| =C-H out-of-plane bending | 1000-600 [2] | - | - | 668 | - | - |
| Si-Si-H _x deformation | 637 [6] | 633 | - | - | - | - |
| Si-P stretching | - | - | - | 494 | 492 | 490 |
| Si-O-Si rocking | 450 [7] | 452 | - | - | - | - |

REFERENCES

[1] Babichev, A.P.; Babushkina, N.A.; Bratkovsky, A.M. Physical quantities. In *Diffusion*; Grigoriev, I.S.; Meilikhov, E.Z., Eds.; Energoatomizdat: Moscow, 1991; pp 375–390.

[2] Stuart, B. H. *Infrared Spectroscopy: Fundamentals and Applications*; John Wiley & Sons: Hoboken, N.J., 2004.

- [3] Tarasevich, B. N. *IR Spectra of Main Classes of Organic Compounds*; Moscow State University: Moscow, 2012.
- [4] Matsumoto, K.; Inada, M.; Umezu, I.; Sugimura, A. *Jpn. J. Appl. Phys.* **2005**, *44*, No. 12, 8742–8746.
- [5] Mendelovici, E.; Villalba, R.; Sagarzazu, A.; Carias, O. *Clay Miner.* **1995**, *30*, 307–313.
- [6] Zhou, S.; Pi, X.; Ni, Z.; Ding, Y.; Jiang, Y.; Jin, C.; Delerue, C.; Yang, D.; Nozaki, T. *ACS Nano* **2015**, *9*, No. 1, 378–386.
- [7] Gunde, M.K. *Physica B* **2000**, *292*, 286–295.