Supporting Information for:

3D microstructure analysis of silicon-boron phosphide mixed nanocrystals

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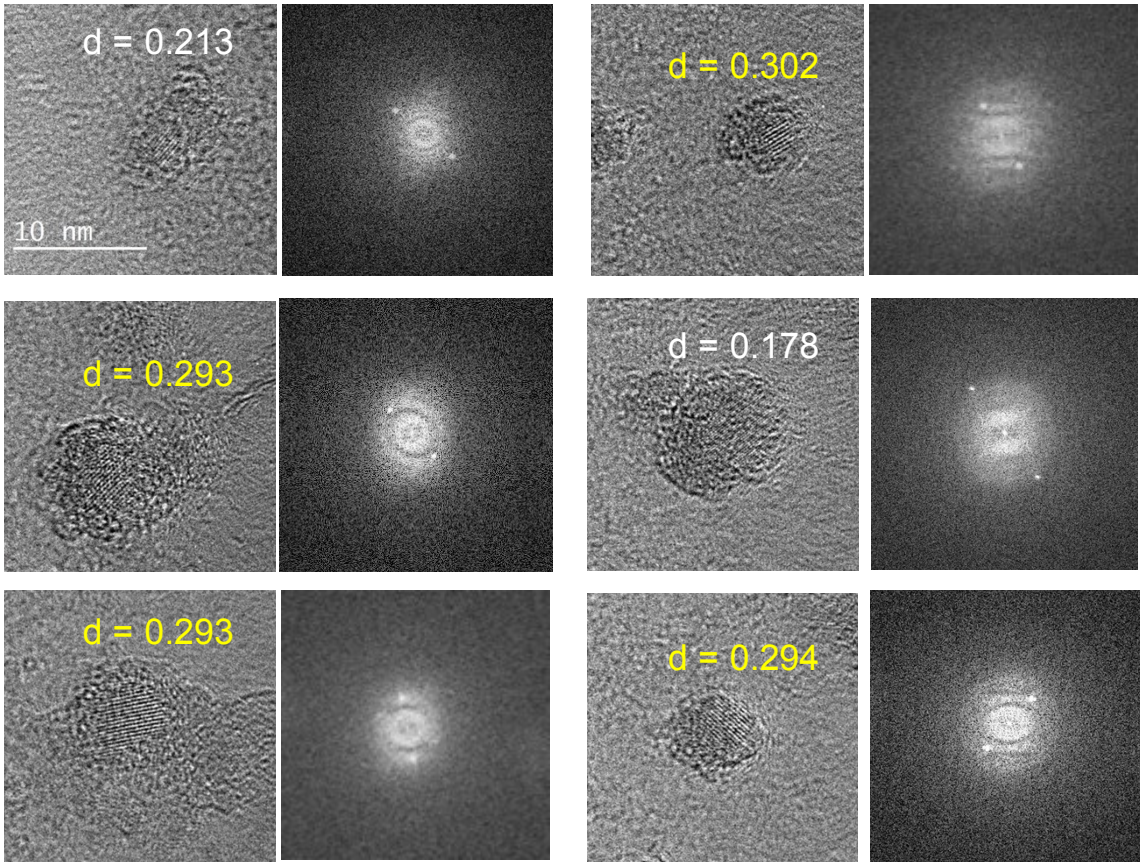

Fig. S1 TEM images and the Fourier transform of $B_xSi_yP_z$ NCs

XPS spectra of $B_xSi_yP_z$ nanocrystals

For XPS measurements of the $B_xSi_yP_z$ nanocrystals, the solutions were drop-cast on gold-coated stainless-steel plates and dense films of nanocrystals formed. XPS measurements were carried out using an Al Kα X-ray source (ULVAC-PHI, PHI X-tool). The detection area was 1.4 mm x 0.1 mm. Therefore, signals from very large numbers of nanocrystals were analyzed and averaged.

Figure S2 provides the XPS spectra of B 1s (P 2s), Si 2p and P 2p peaks. XPS spectra exhibiting high signal-to-noise ratios were obtained. The atomic ratios of the B, P and Si were estimated from integrated intensities of the peaks by taking into account the ionization cross-sections of each element. Unfortunately, the XPS signal of B 1s is overlapped with that of P 2s. Therefore, we subtracted the contribution of the P 2s signal from the spectrum in Figure S2(a) by the following procedure. First, the intensity ratio of P 2s signal (I'_{P2s}) to P 2p signal (I'_{P2p}) of a standard phosphorous sample (red phosphorus) was measured (I'_{P2s}/ I'_{P2p}). The intensity of P 2s signal (I_{P2s}) was then calculated by multiplying I'_{P2s}/ I'_{P2p} to that of P 2p signal (I_{P2p}) obtained from Figure

S2(c) ($I_{P2s} = I_{P2p}$ x (I'_{P2s}/ I'_{P2p})). Finally, I_{P2s} was subtracted from the integral intensity of the spectrum in Figure S2 (a) to obtain the B 1s signal intensity.

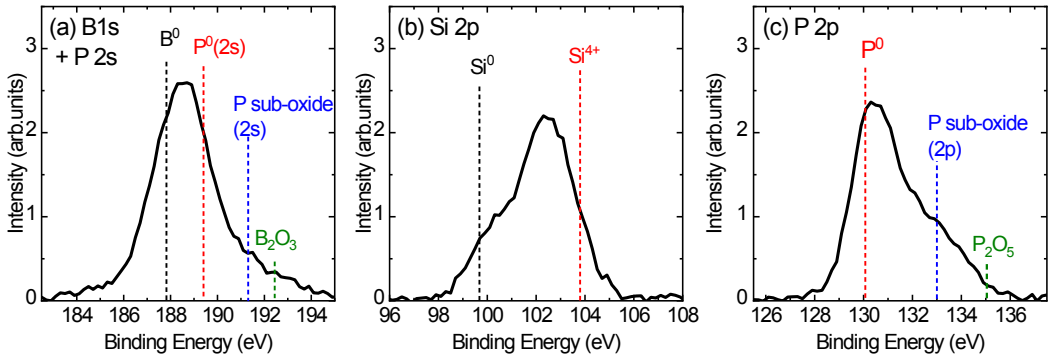

Fig. S2 (a) B1s (P 2s), (b) Si 2p and (c) P 2p XPS spectra of $B_xSi_yP_z$ NCs grown at 1200 °C.

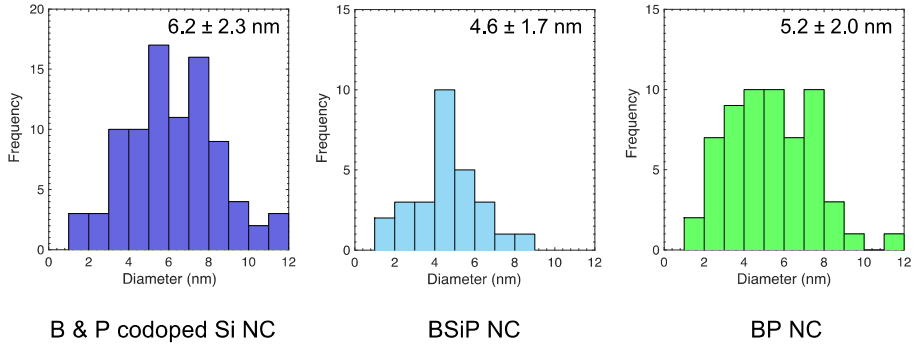

Fig. S3 Size distributions of B and P codoped Si NCs, $B_xSi_yP_z$ NCs, and BP NCs obtained from APT 3D reconstructions.

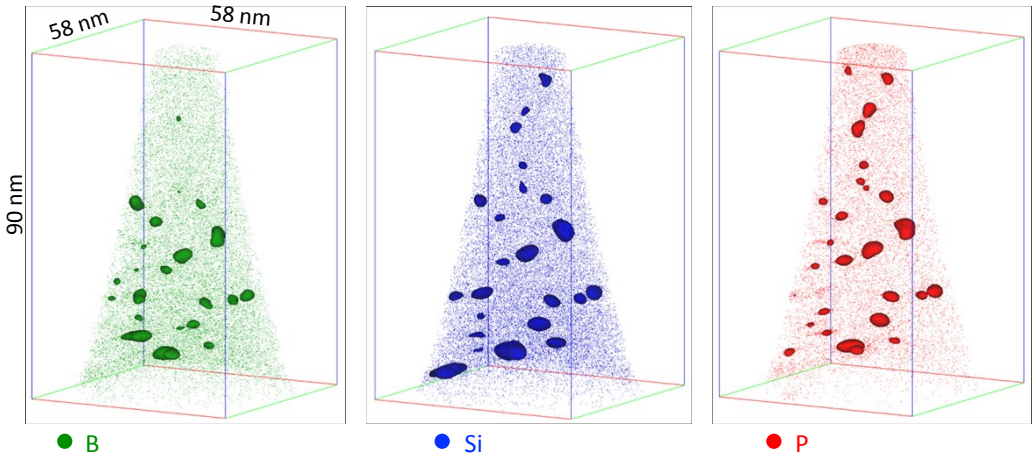

Fig. S4 APT reconstructions of $B_xSi_yP_z$ NCs. Iso-density surface of B, Si and P is 2 atoms/nm^3, 14 atoms/nm^3, and 2 atoms/nm^3 respectively.

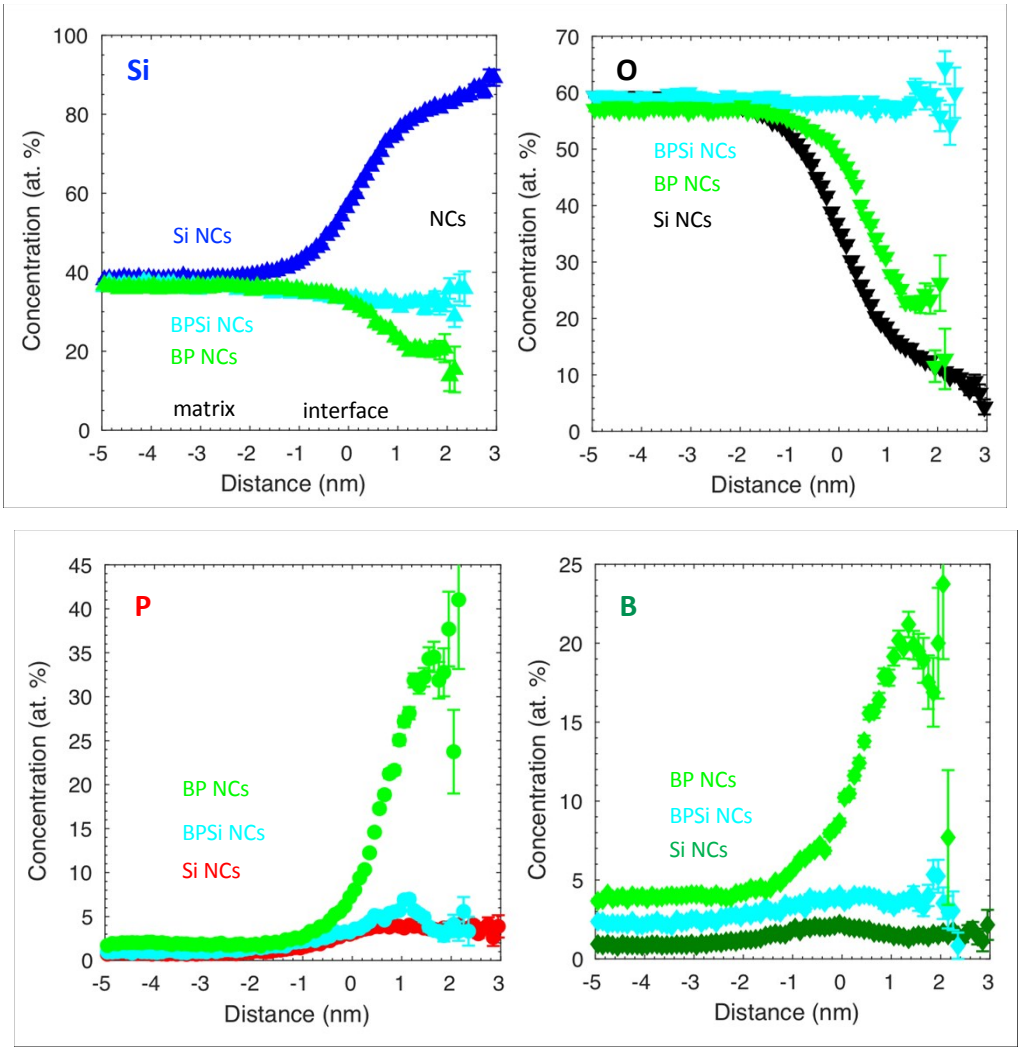

Fig. S5 Si, O, P and B profiles for B and P codoped Si NCs, $B_xSi_yP_z$ NCs, and BP NCs.

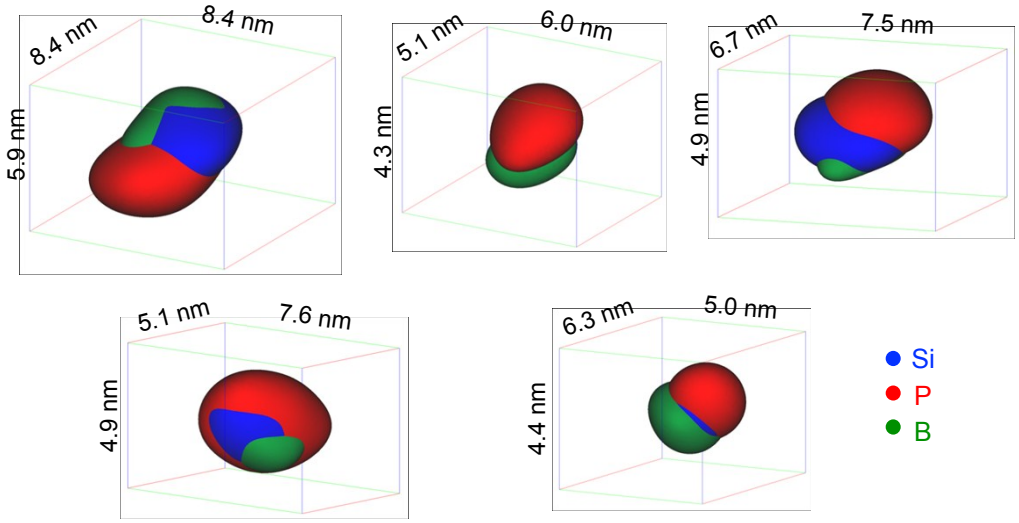

Fig. S6. APT reconstructions of individual $B_xSi_yP_z$ NCs. The voxel size used here is 0.1 nm.

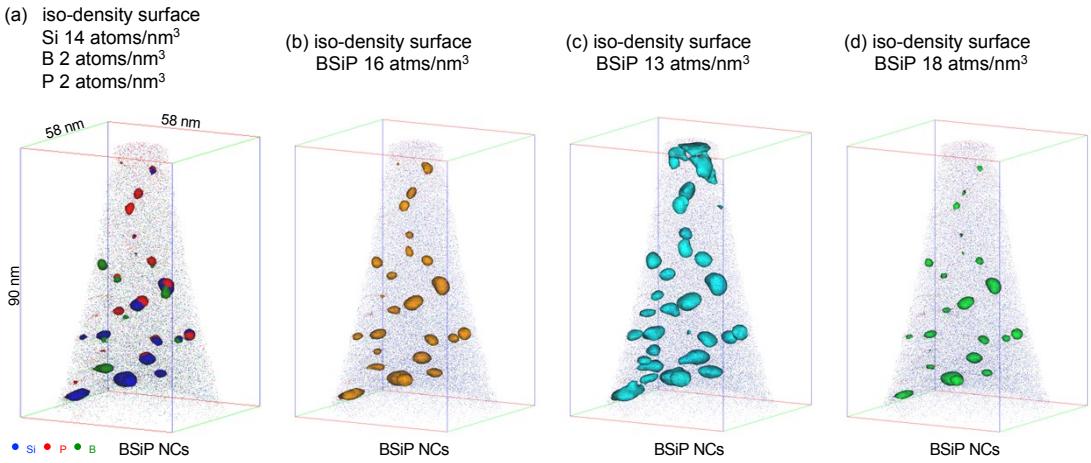

Fig. S7. APT reconstructions of $B_xSi_yP_z$ NCs with different iso-density surfaces. (a) the same as Figure 3(b) in the main text, (b-d) $B_xSi_yP_z$ NCs created by the iso-density surface values of 16 atoms/nm^3 (b), 13 atoms/nm^3 (c), and 18 atoms/nm^3(d).

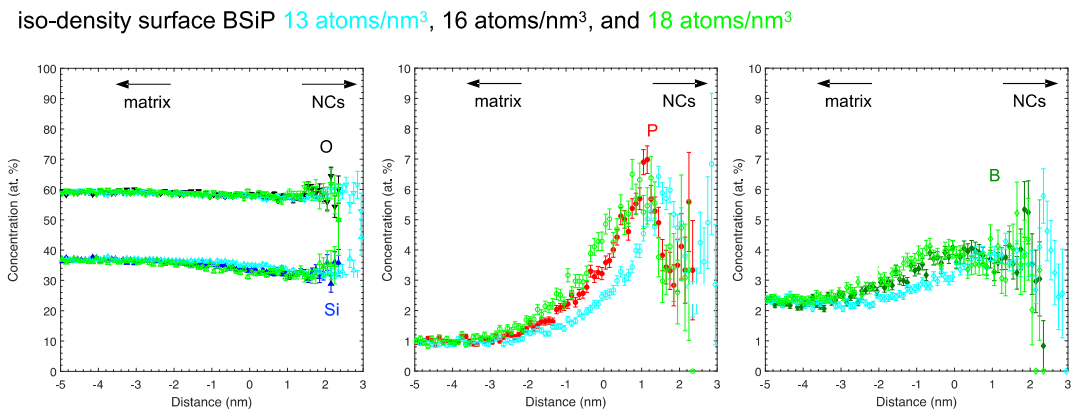

Fig. S8. Proxigram profiles of $B_xSi_yP_z$ NCs created by the iso-density surface values of 16 atoms/nm^3, 13 atoms/nm^3, and 18 atoms/nm^3.

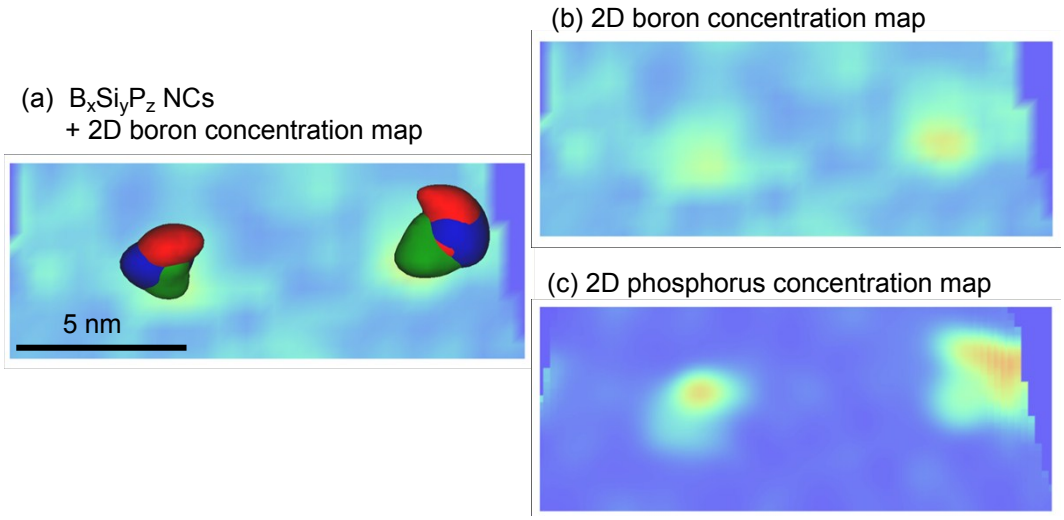

Fig. S9. 2D concentration mapping of B and P atoms. (a) $B_xSi_yP_z$ NCs + 2D B concentration map, (b) 2D B concentration map, and (c) 2D P concentration map.