Supporting Information for

Retarded Dopant Diffusion by Moderated

Dopant-Dopant Interactions in Si Nanowires

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Fig. S1. Formation energy changes with the number of unit cell along axial direction for 2.5 nm [110] SiNWs.



Fig. S2. Atomic configurations when the 2 B are located at (a) Cen-Cen (Center and Center), (b) Cen-SS (Center and Sub-surface), and (c) SS-SS (2 Sub-surface sites). (d) The 3 B exist at SS-SS-SS (3Sub-surface sites). Boron atoms are represented with pink ball.



Fig. S3. The charge density profile of valence band maximum of the nearest 2 B case (B is at a1 in Fig. 1b) shows different correlation with that of the farthest 2 B case (B is at a3 in Fig. 1b)



Fig. S4. Si slab structure used for the formation energy calculation.