Supporting information for:

How Big Does a Si Nanocluster Favor Bulk Bonding Geometry?

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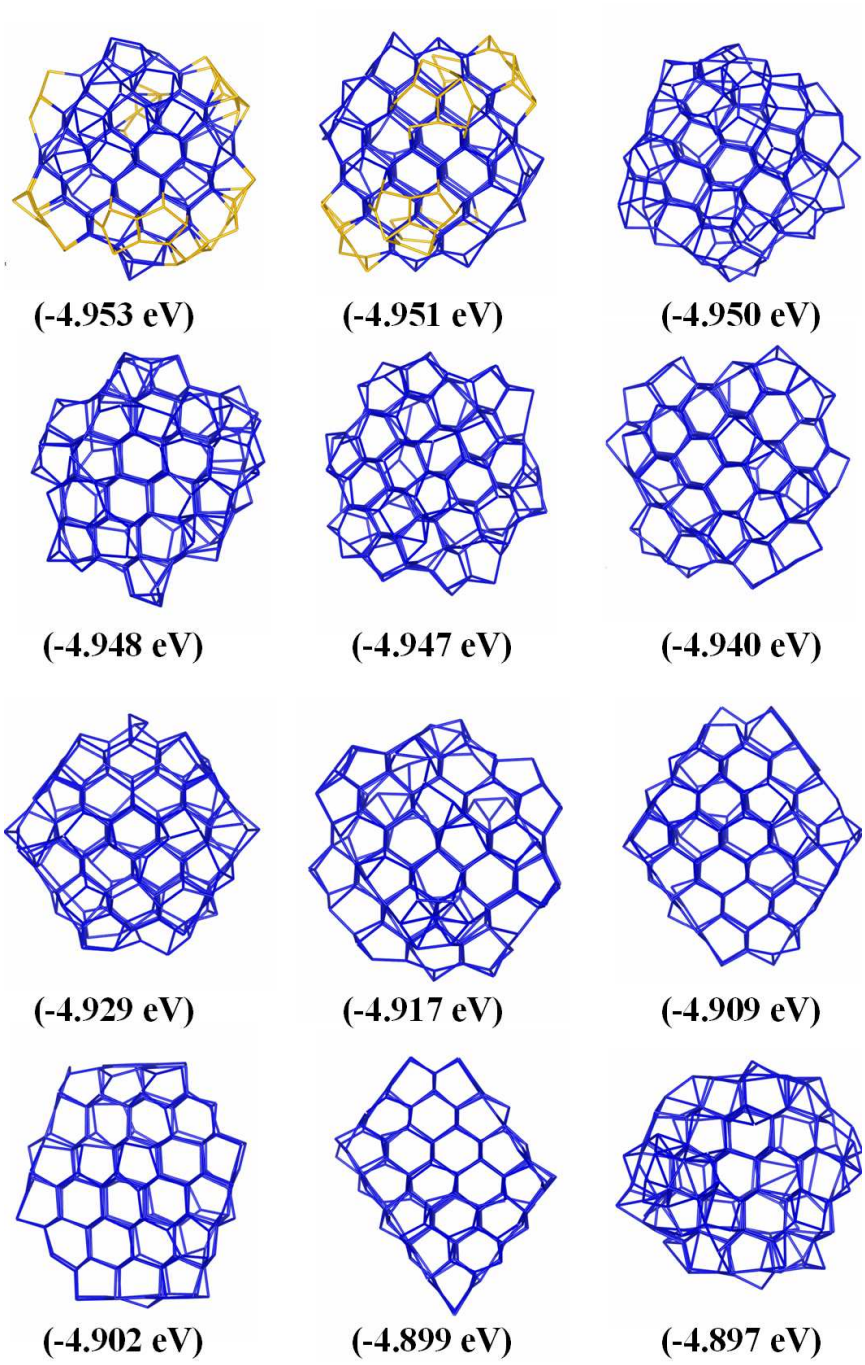

Figure S1: Structures of the bulk-like Si_{220} NCs. The values in brackets are the DFT-PBE cohesive energies per atom. The surface and bulk-like Si atoms were denoted by yellow and blue colors, respectively.

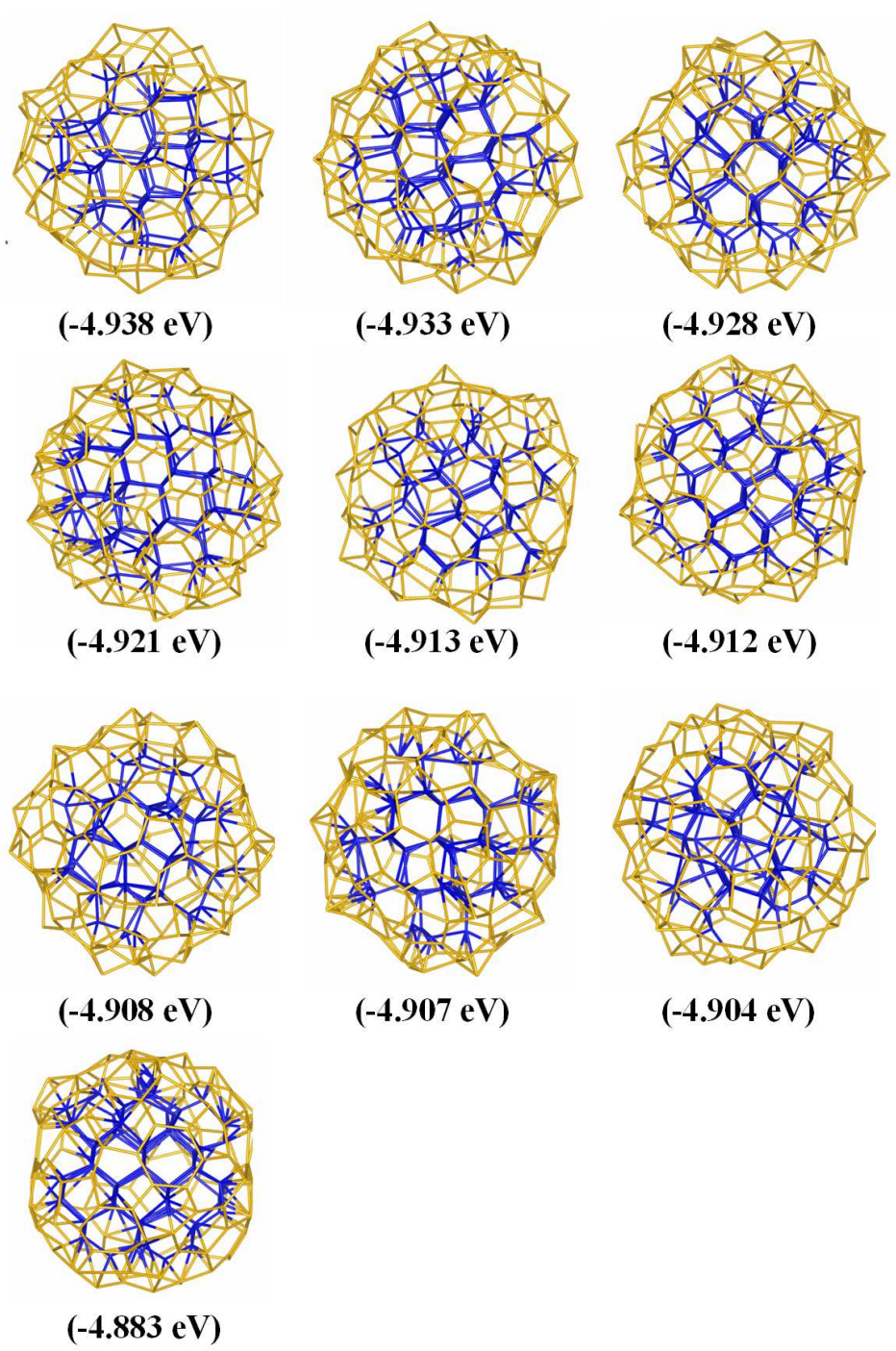

Figure S2: Structures of the bucky-diamond Si_{220} NCs. The values in brackets are the DFT-PBE cohesive energies per atom. The surface and core atoms were denoted by yellow and blue colors, respectively.

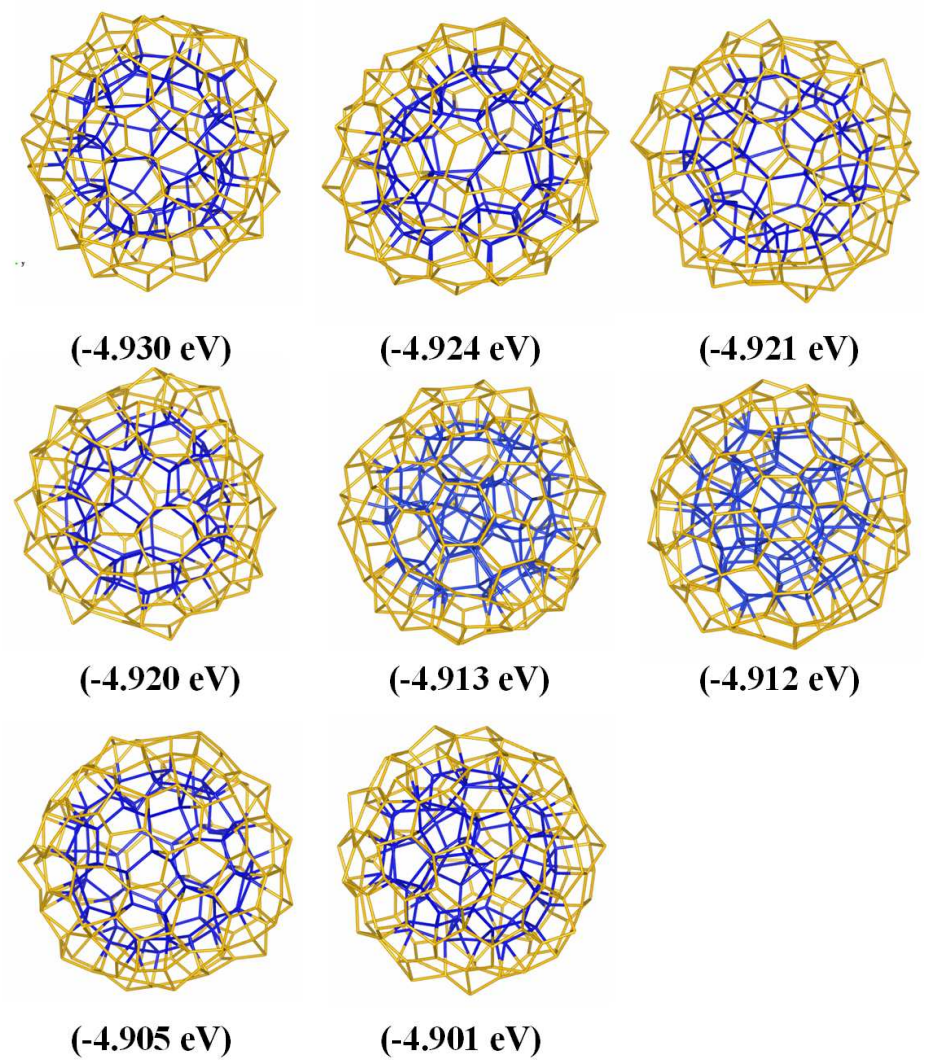

Figure S3: Structures of the onion-like Si_{220} NCs. The values in brackets are the DFT-PBE cohesive energies per atom. The surface and core atoms were denoted by yellow and blue colors, respectively.