Supplementary Information (SI) for Physical Chemistry Chemical Physics.

Modulating Electronic Properties in Hydrogenated Silicon Nanotubes

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Supplementary Materials

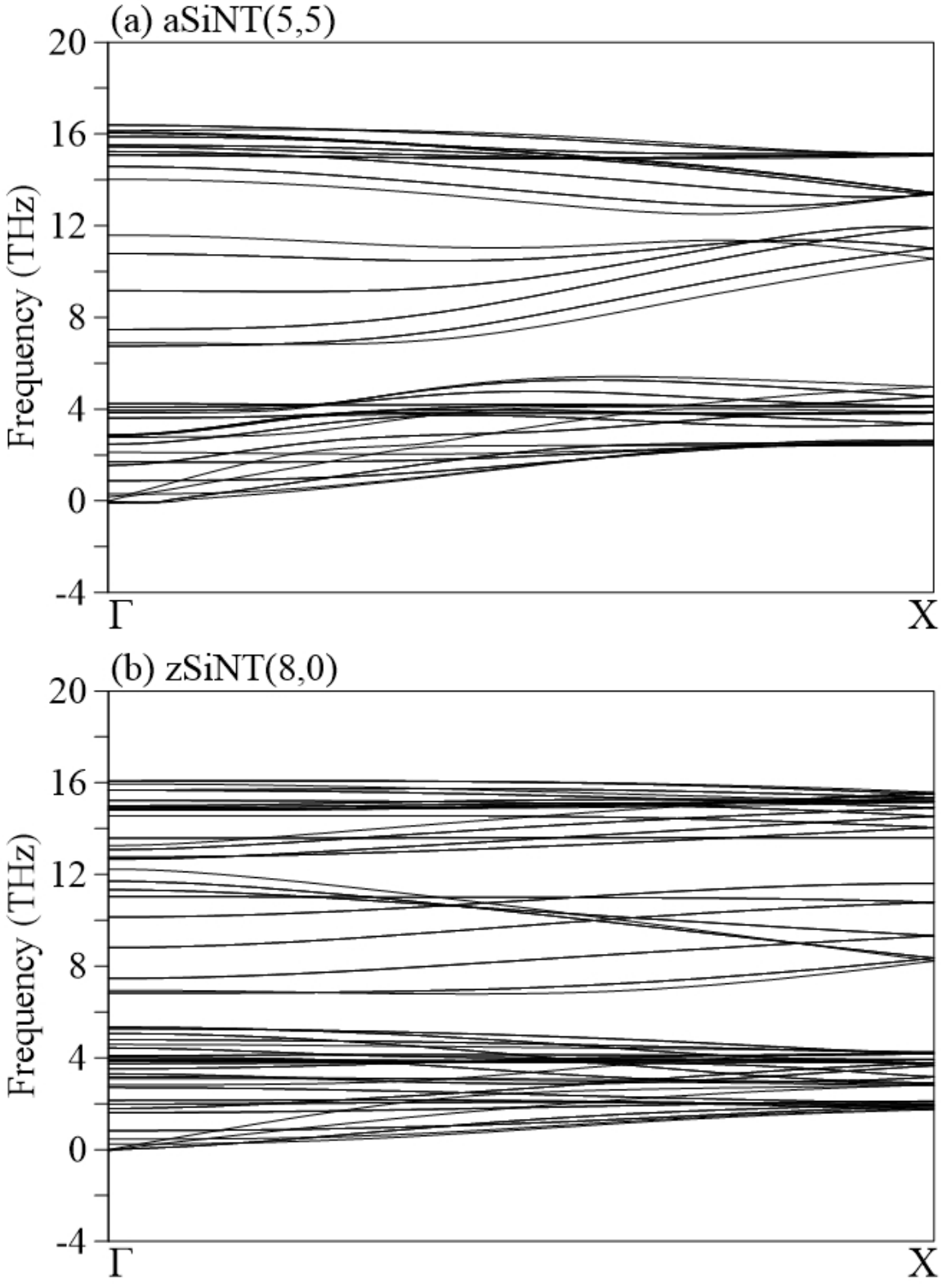

Figure S1: Phonon spectra of (a) aSiNT(5,5) and (b) zSiNT(8,0).

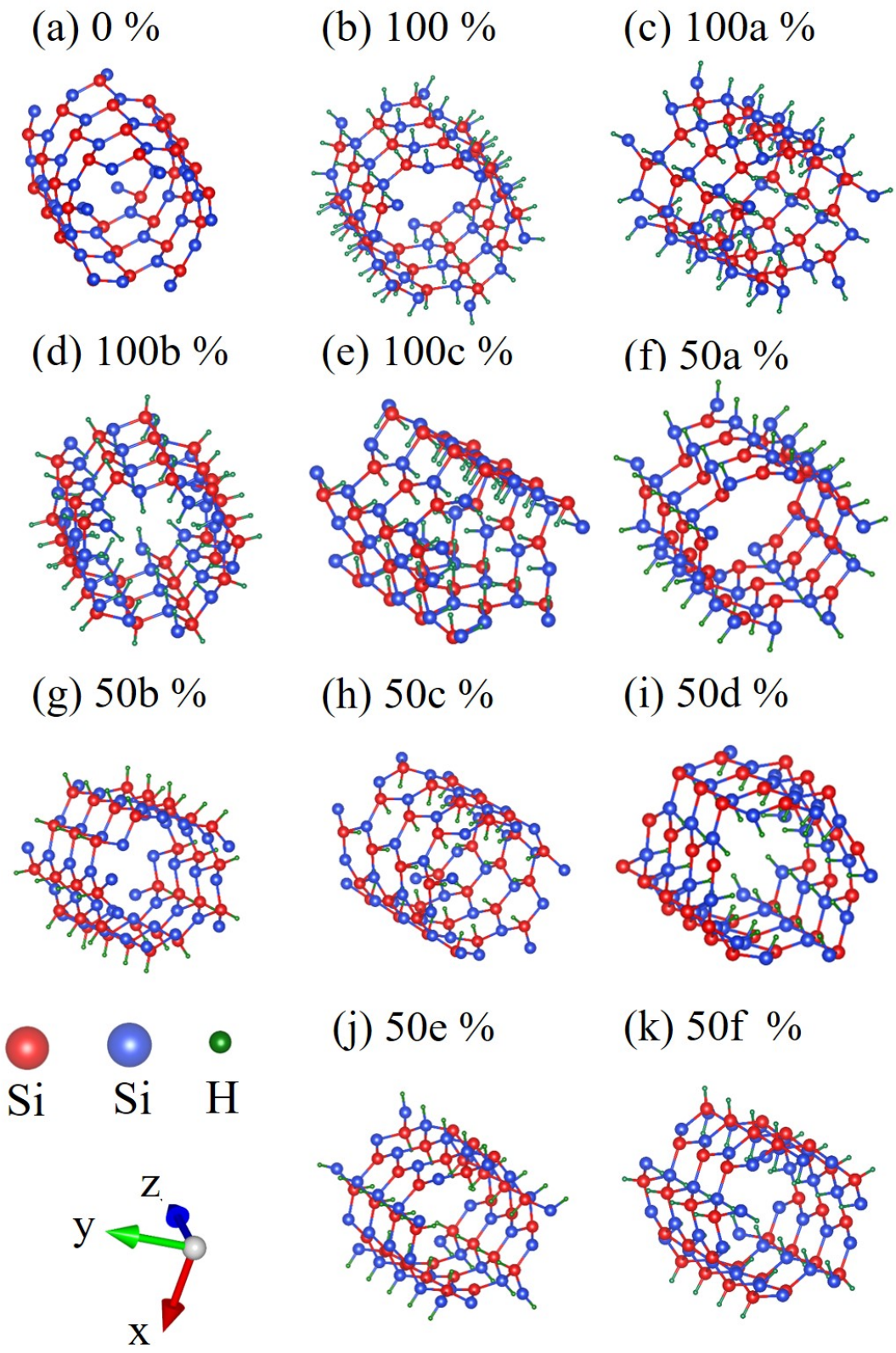

Figure S2: Tilted views of (a) pure and (b)-(k) hydrogenated Si(5,5) NTs with various adsorption types and concentrations.

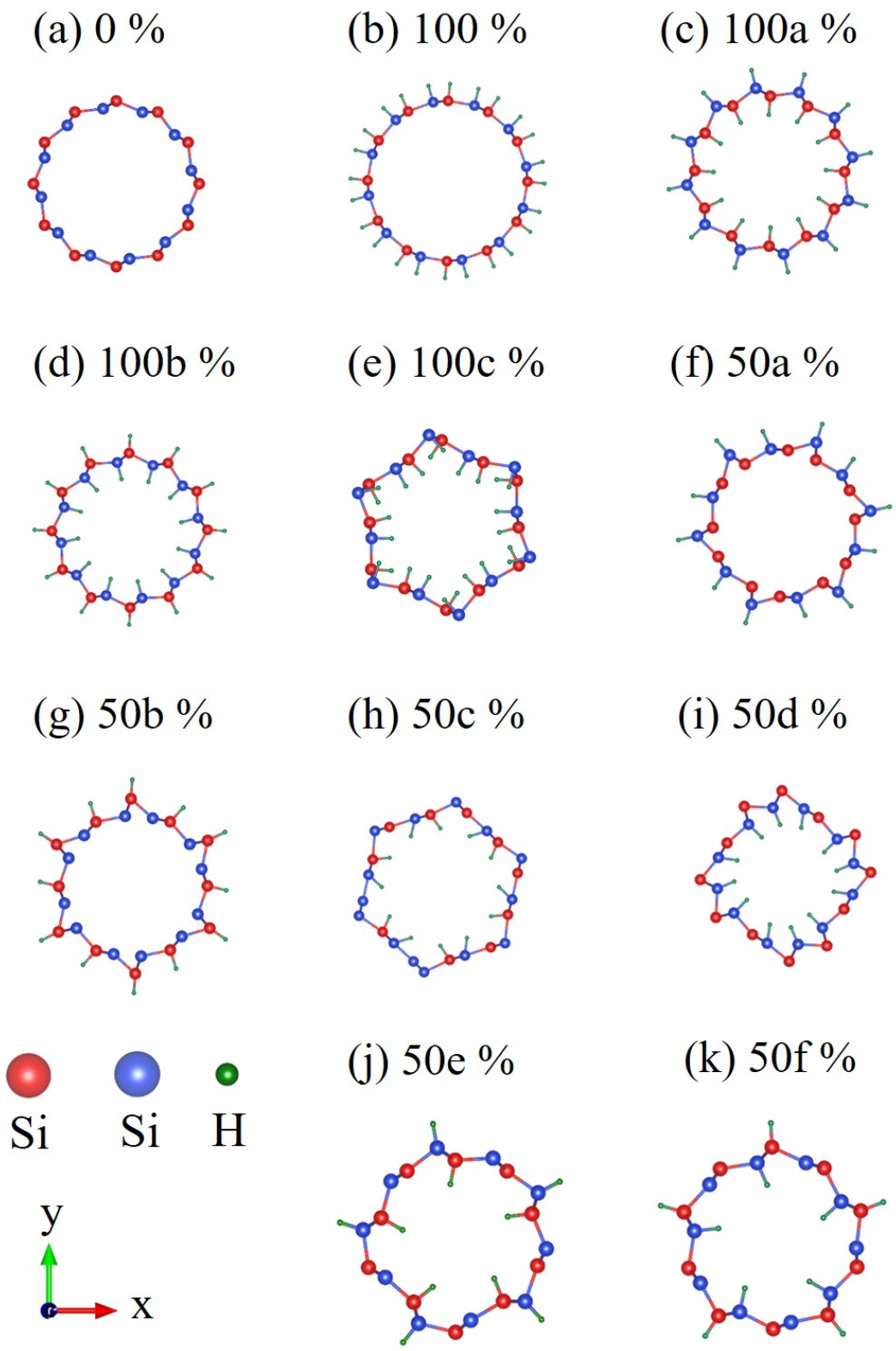

Figure S3: Cross-sectional views of (a) pure and (b)-(k) hydrogenated Si(6,6) NTs with various adsorption types and concentrations.

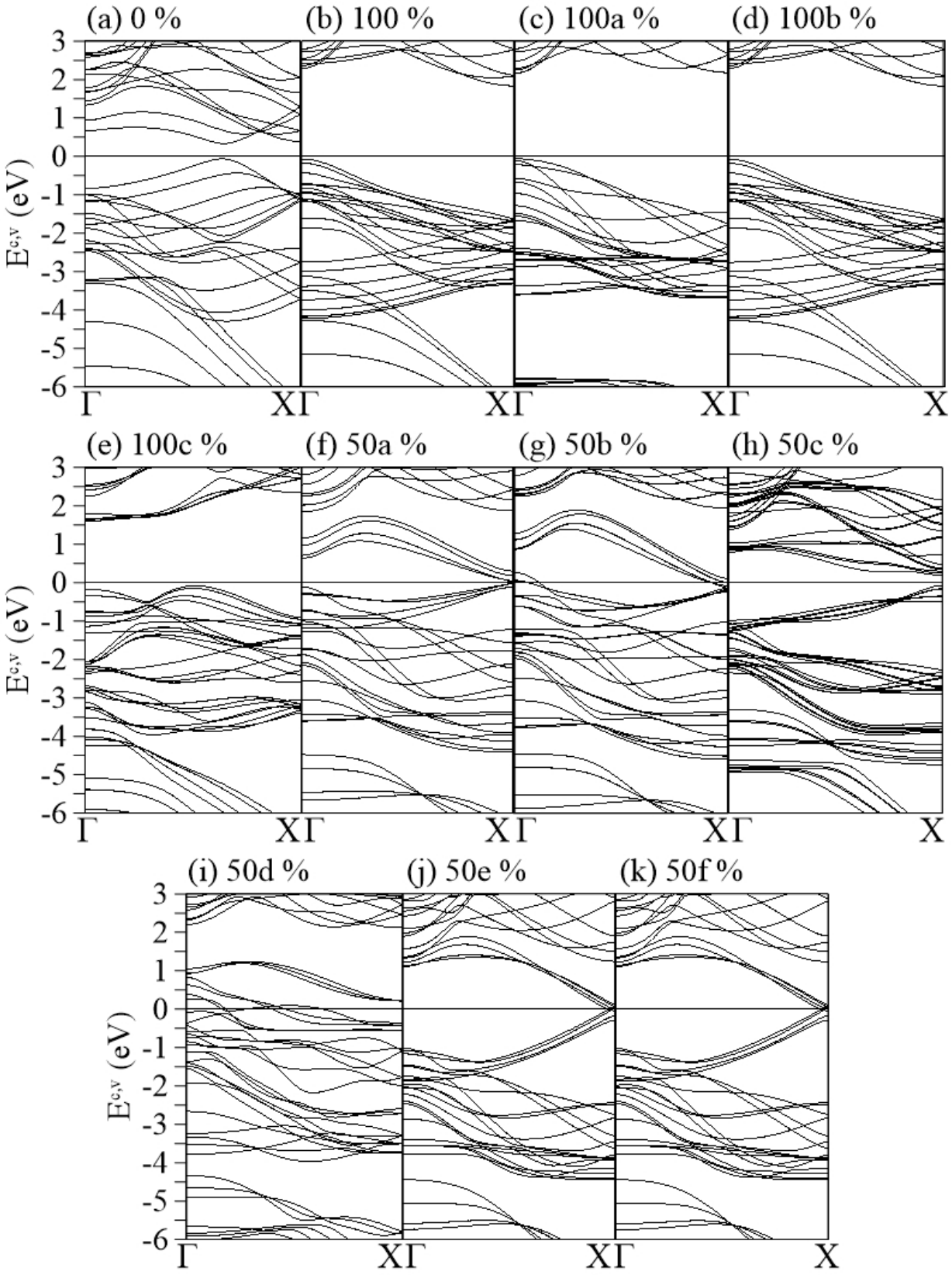

Figure S4: Band structures of (a) pure and (b)-(k) hydrogenated Si(6,6) NTs with various adsorption types and concentrations.

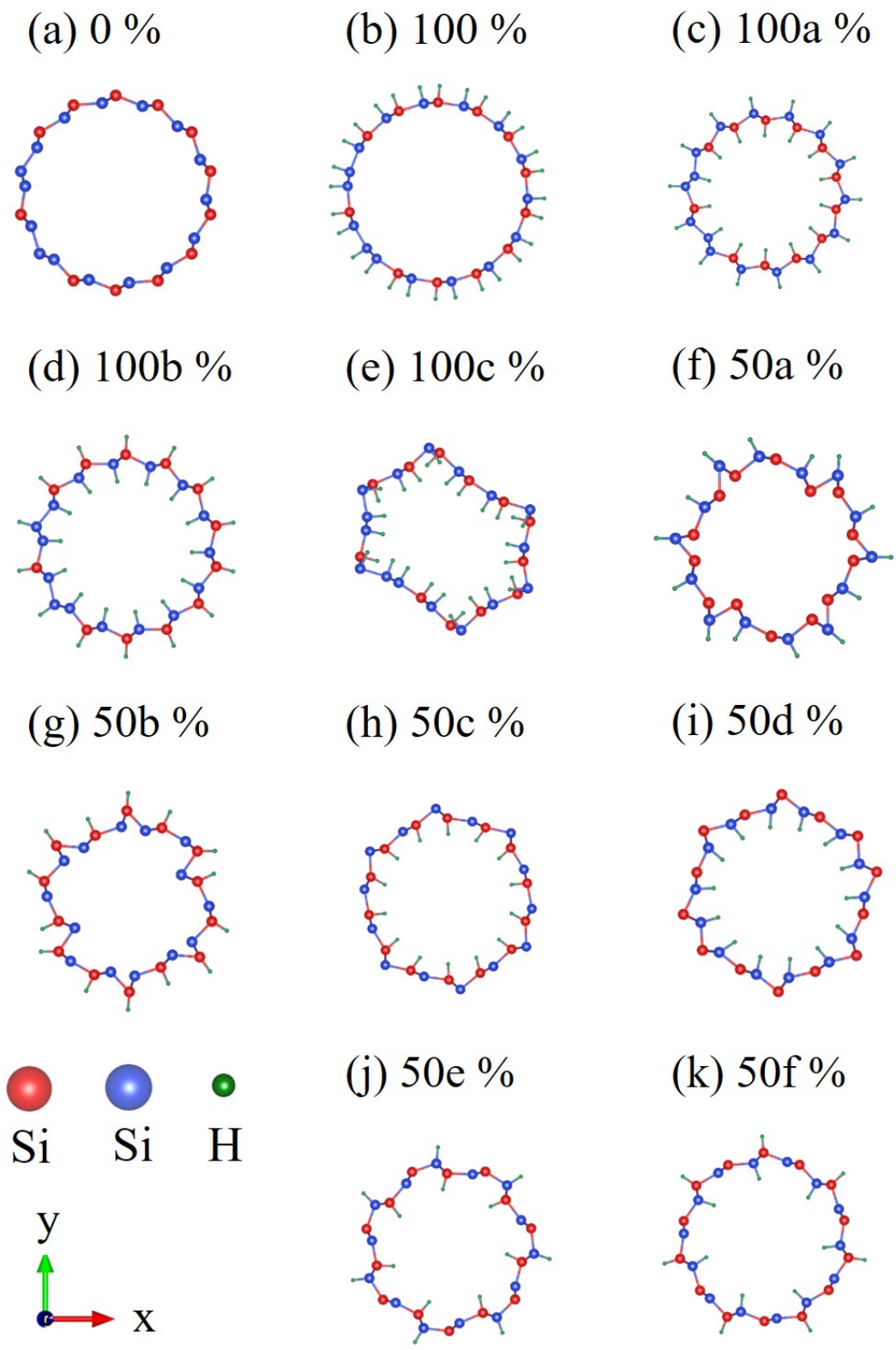

Figure S5: Cross-sectional views of (a) pure and (b)-(k) hydrogenated Si(7,7) NTs with various adsorption types and concentrations.

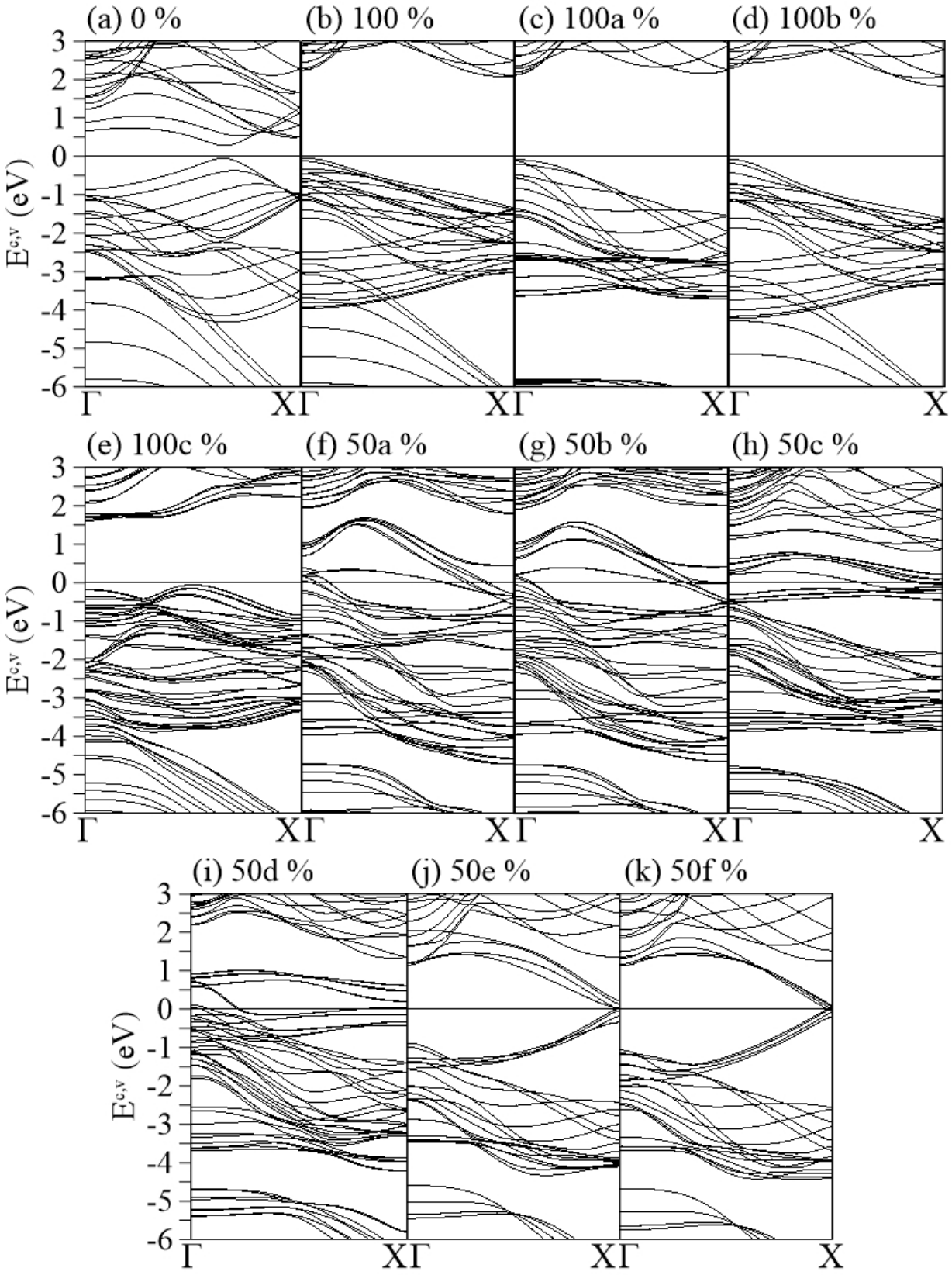

Figure S6: Band structures of (a) pure and (b)-(k) hydrogenated Si(7,7) NTs with various adsorption types and concentrations.

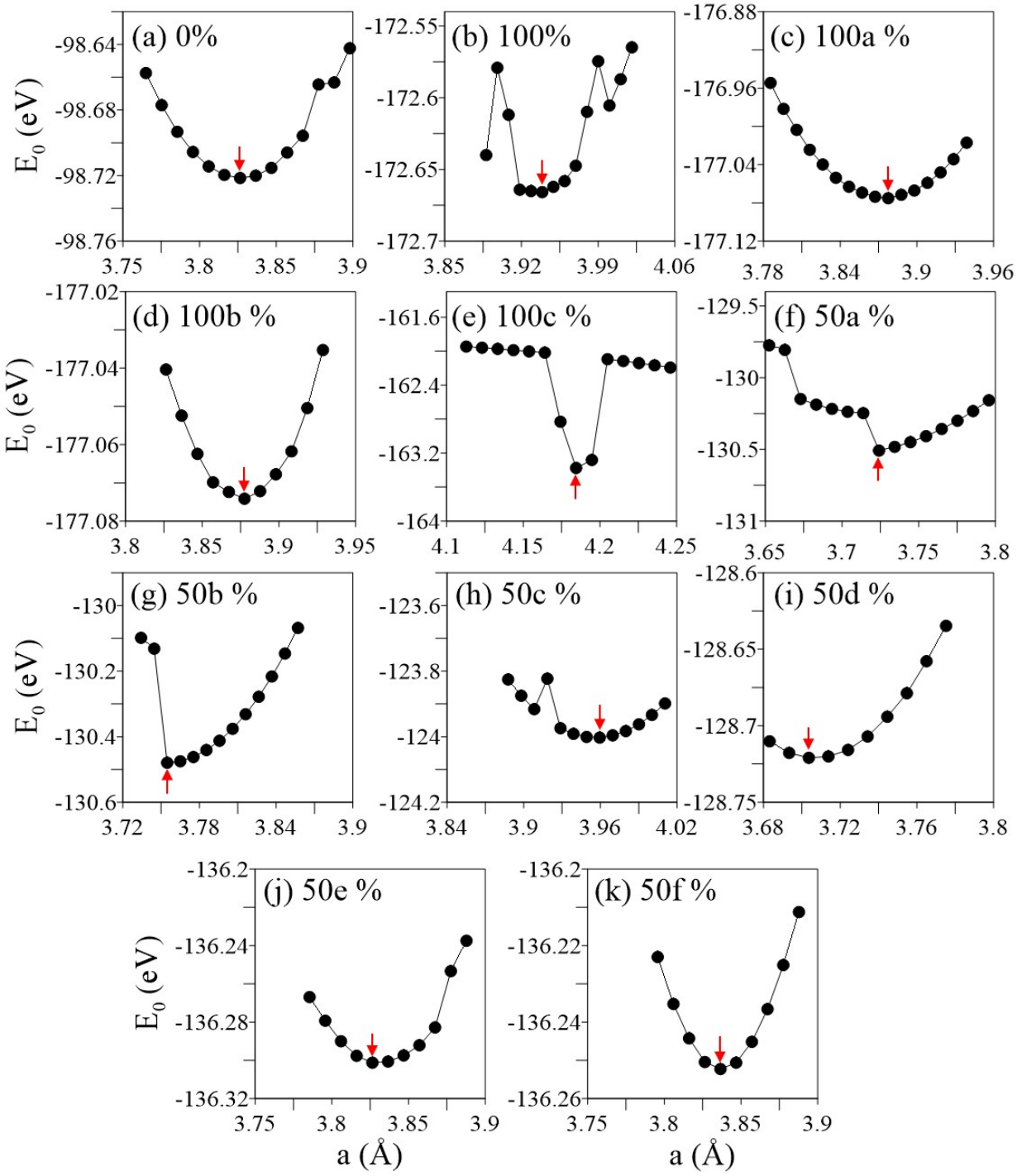

Figure S7: The lowest total energy E_0 as a function of the lattice constant "a" for (a) pure and (b)-(k) hydrogenated Si(5,5) NTs with various adsorption types and concentrations. Red arrows indicate the minimum E_0 for each case.