Electronic Supplemental Information for

Embedded Silicene Nanostructures in Partly-Dehydrogenated Polysilane

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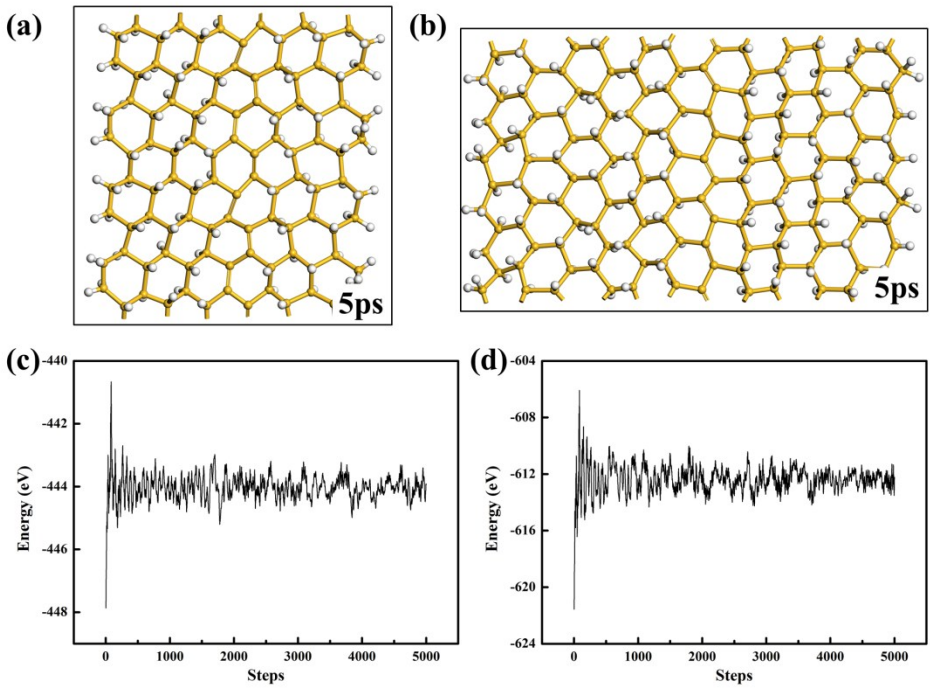

Figure S1. Born-Oppenheimer molecular dynamic simulation for (a) *E*-1-ASiNR and (b) *E*-1-ZSiNR, respectively. The simulated temperatures of systems maintain at 500 K. The time step is 1 fs and the total simulation time is 5 ps. (c) Energy curve of *E*-1-ASiNR during simulation. (d) Energy curve of *E*-1-ZSiNR during simulation.

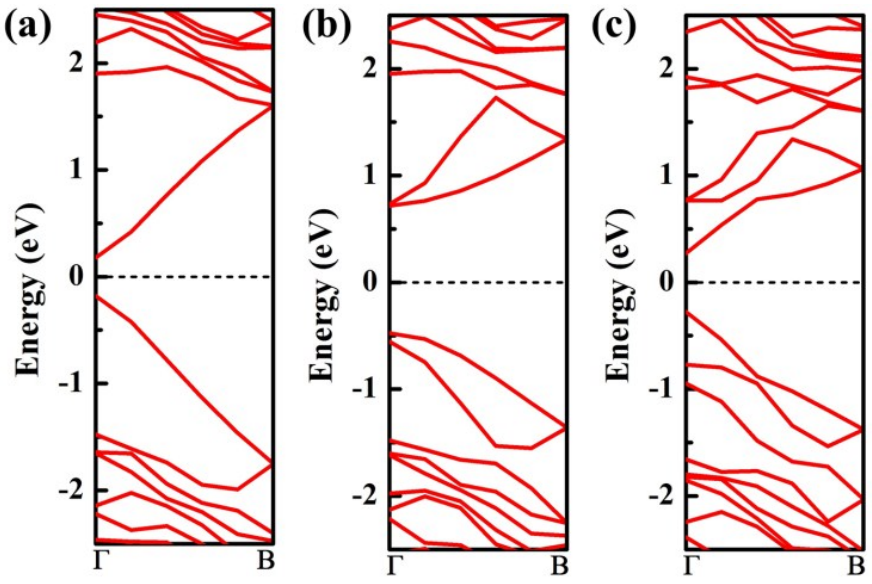

Figure S2. Calculated band structure of embedded armchair-edged silicene nanoribbons based on the HSE06 method for (a) E-1-ASiNR, (b) E-2-ASiNR and (c) E-3-ASiNR, respectively.