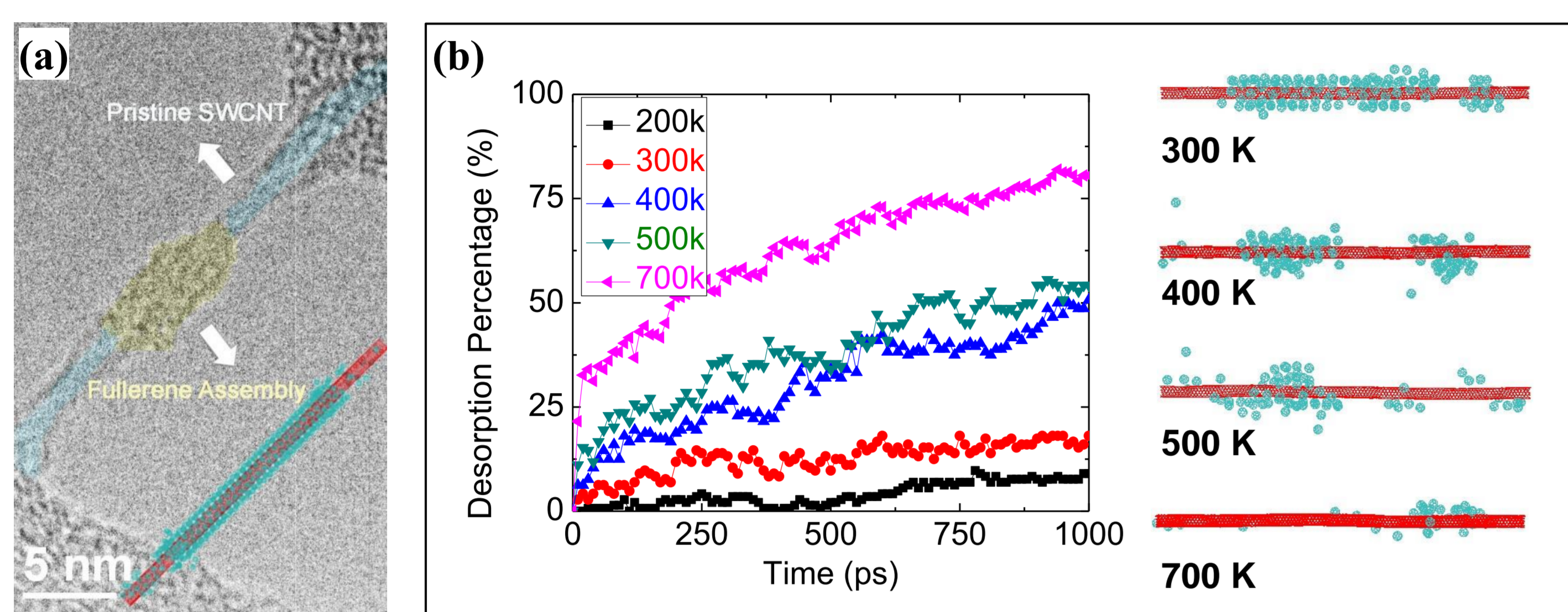


Self-assembly of All-carbon Core-shell Nanostructures for Photovoltaics

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Abstract: Using a complementary experiment and molecular dynamics simulation approach, we show that p-type semiconducting carbon nanotubes (s-SWCNTs) and n-type C_{60} s can form radial p-n junctions by geometrically driven co-assembly with graphene nanoribbons (GNRs). The resulting core/shell like structure greatly emulate the 1-D nanowire with enhanced structural stability, making them well suited for for photovoltaic applications.

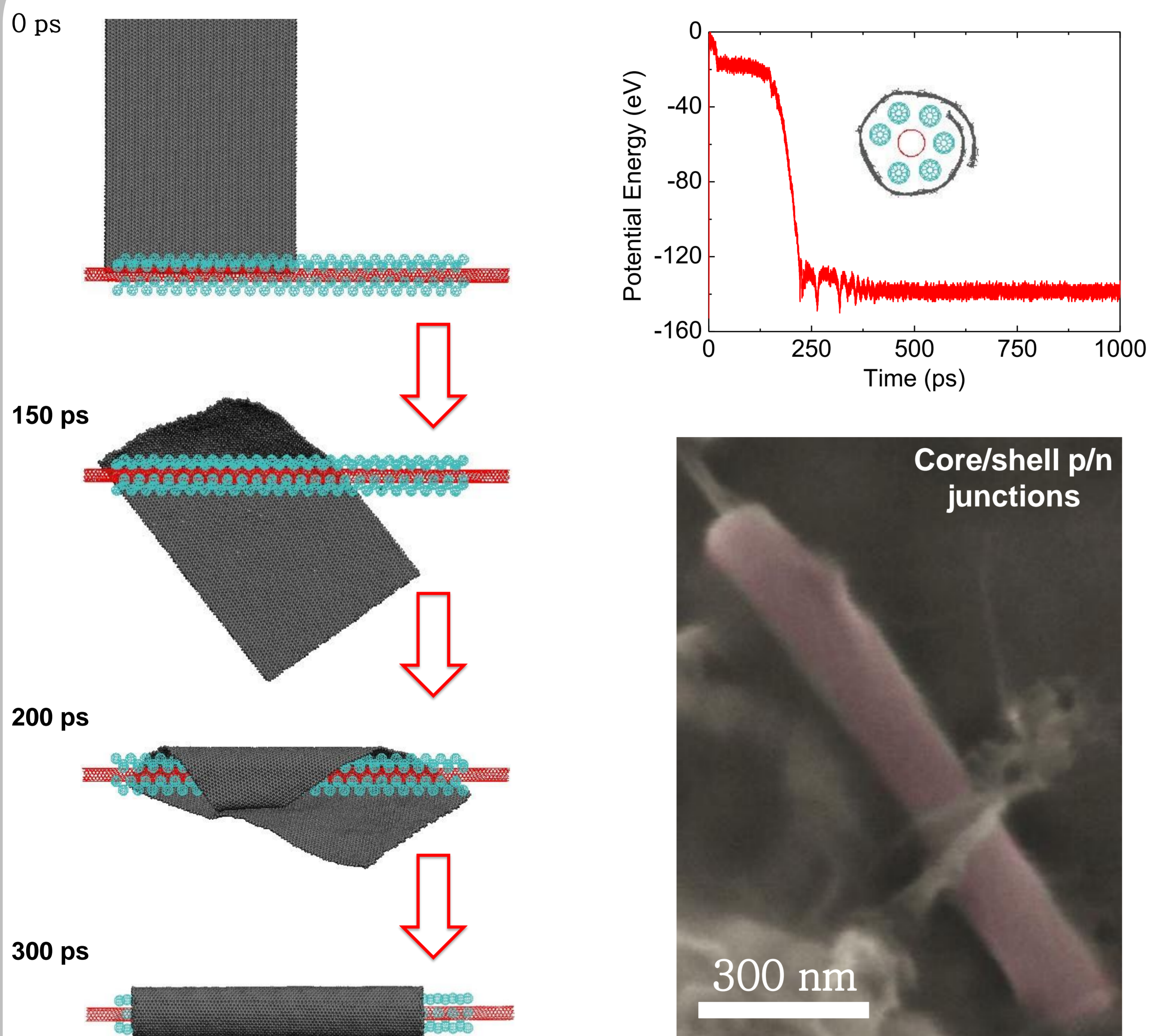
I. All-carbon Core/shell Structures and Stability



(a) Our experimental result and molecular dynamics simulations collectively show that C_{60} s can coat the surface of s-SWCNT surfaces, forming radial p-n junctions

(b) Increasing temperature decreases the stability of the structure which is undesirable for device performance; instability is characterized by the percentage of C_{60} molecules desorbed from the CNT surface

II. Graphene Wrapping



To stabilize the core-shell structure, we utilized graphene nanoribbons (GNRs) to wrap the s-CNT/ C_{60} hybrids such that the C_{60} molecules are trapped next to CNT. The process was demonstrated by both molecular dynamics simulations and experiments; typical images are shown above. The model predicts that potential energy decreases during the wrapping process, indicating that wrapping is energetically favorable.

Acknowledgement:

We thank Professor Jiaying Huang, Professor Mark C. Hersam and Jaemyung Kim of Northwestern University for their help and discussions.

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III. Energetic Analysis in the Wrapping Process

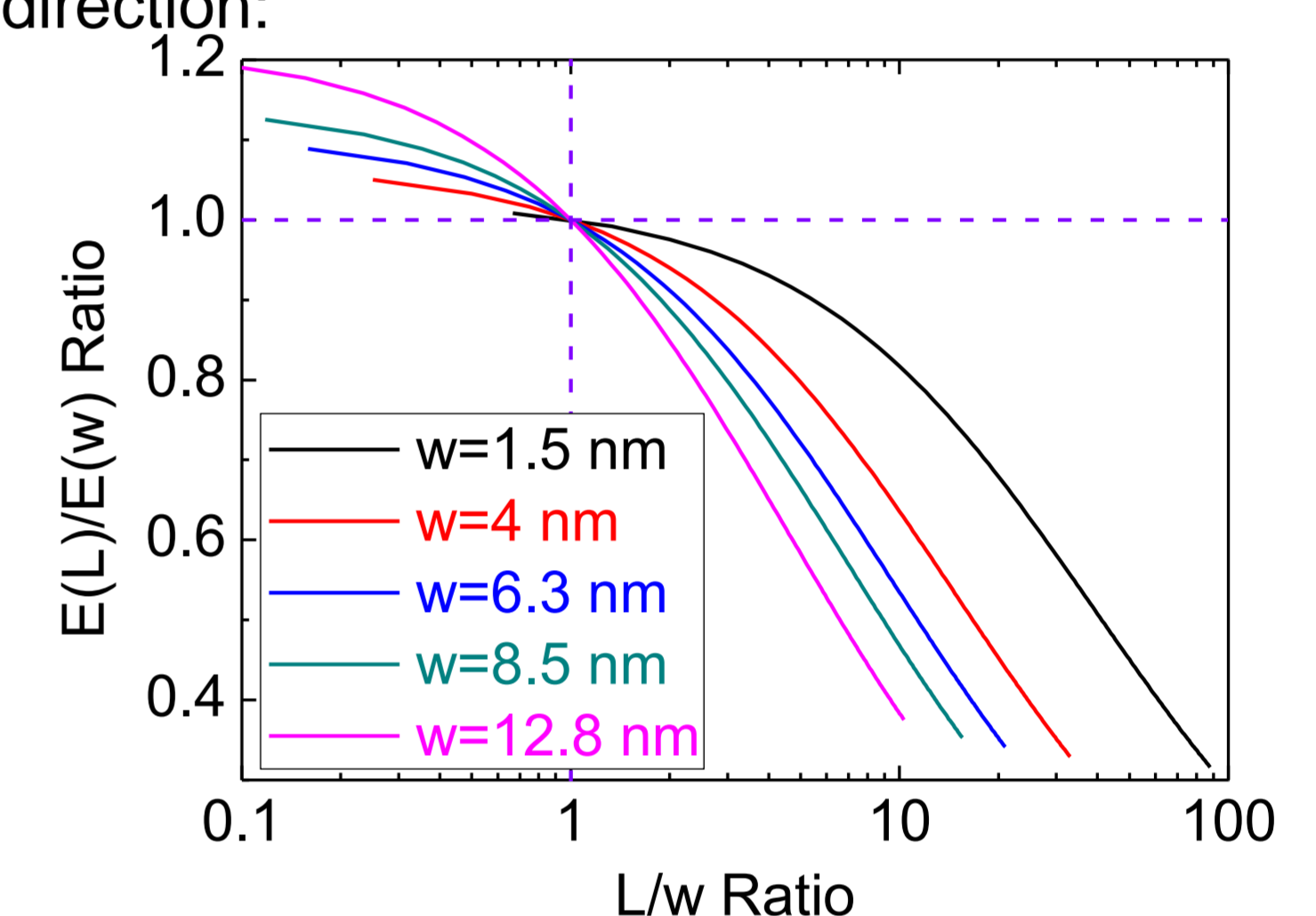
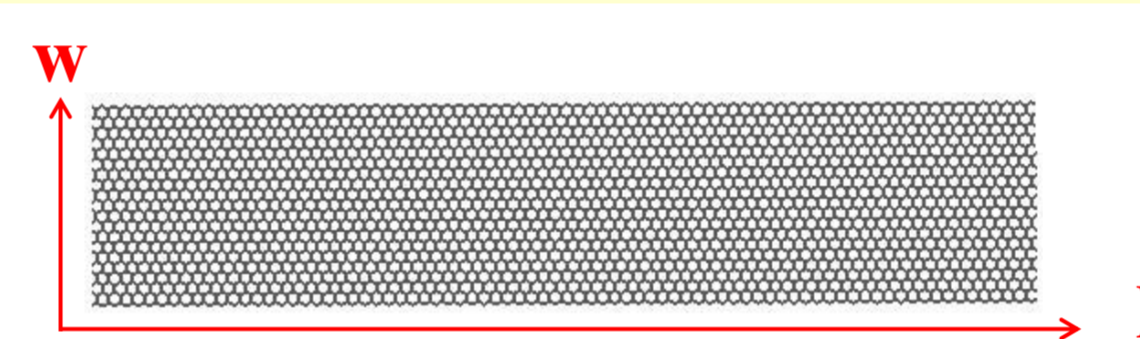
GNR geometry is defined by their length and width. We analyzed how these features affect the wrapping process. We investigated the energetic contributions involved in the process: van der Waals energy and bending energy:

$$E = E_{vdw} + E_{bending} = -0.01785Lw + \frac{2\rho Dw}{3.4 + \frac{2\rho(R+13.5)^2}{L}}$$

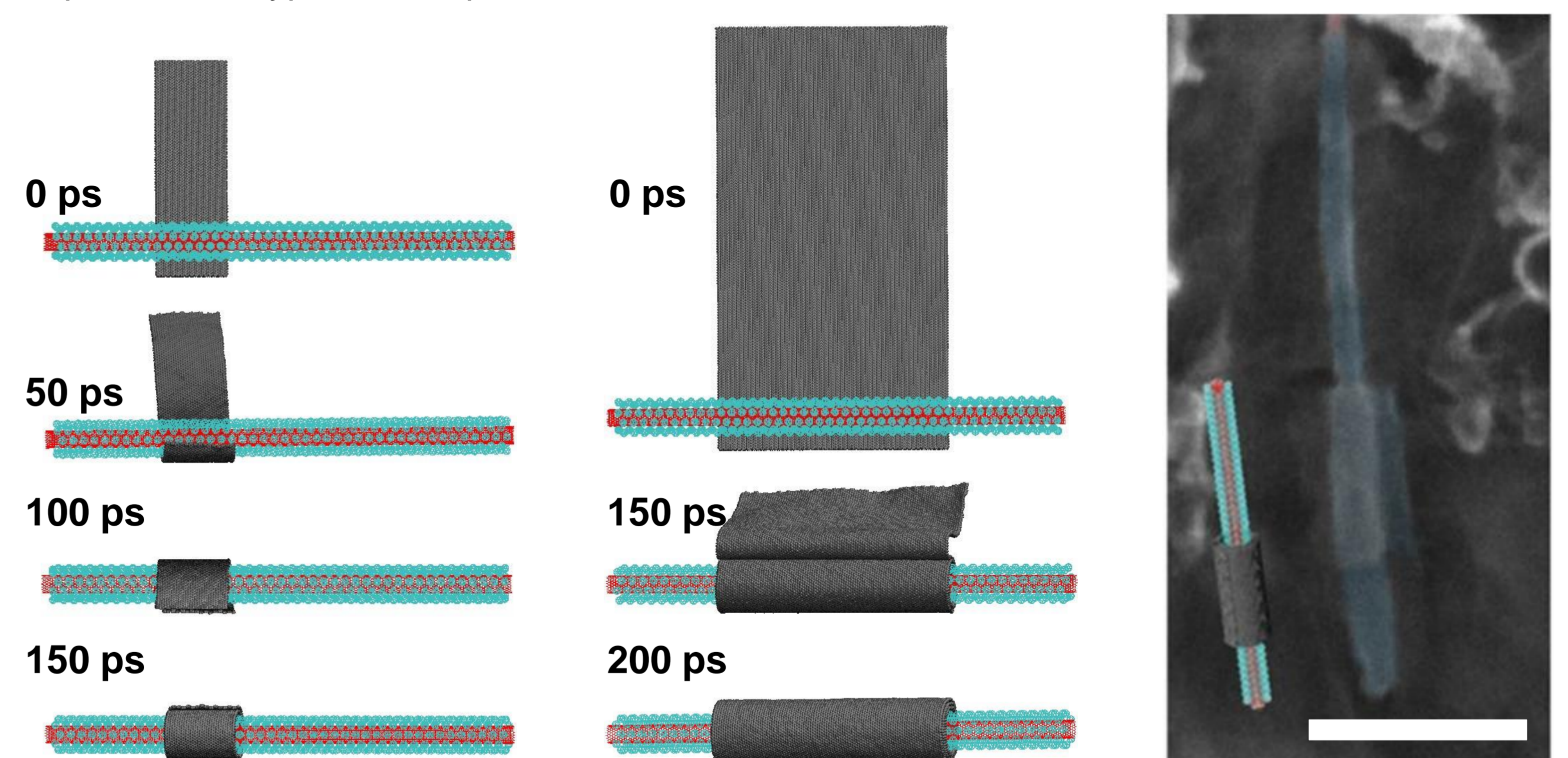
L: length of the ribbon, w: width
 D: bending stiffness of the GNR
 R: carbon nanotube radius

This equation indicates that van der Waals energy encourages the wrapping process while the bending energy resists wrapping. This can be used to predict the direction wrapping will occur since the system will proceed in the direction that costs the lowest bending energy. The two extremes are along the L direction and w direction:

$$\frac{E_{bending}(L)}{E_{bending}(w)} = \frac{3.4w + 2\pi(R+13.5)^2}{3.4L + 2\pi(R+13.5)^2}$$



The energy ratio as a function of L/w ratio is shown above. It indicates that wrapping along the L direction is preferred; this is consistent with observations from the simulations and experiments. Typical examples are shown below:



IV. Improved Stability

After the wrapping process is completed, the structural stability of the multi-core-shell structure is significantly improved, as evidenced by our simulations at high temperatures.

A longitudinally wrapped structure (a) is subjected to a temperature of 500 K (b). The C_{60} molecules wrapped by the GNR remain in their original lattice arrangement (the bottom image in (b) is from the same snapshot but with the GNR not shown). The cross-section view in (c) clearly indicates that the wrapping pattern is not affected by the high temperature stimulation.

This improved structural stability of s-CNT/ C_{60} radial p-n junction makes them promising candidates for a new generation of all-carbon solar cell applications.

