Forming a graphdiyne nanotube from a nanoribbon through heat treatment in a protective gas: A molecular dynamics study

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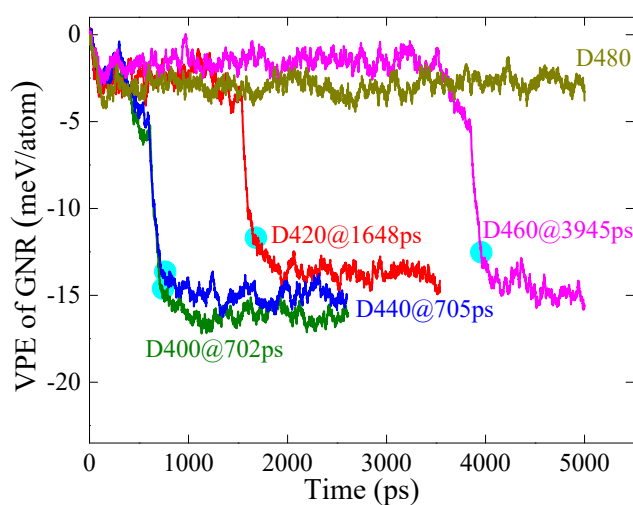

Fig. A.1. VPE per atom of the GNR self-scrolling on CNT (15, 15) in argon within D400 to D480 at 300 K vs the simulation time.
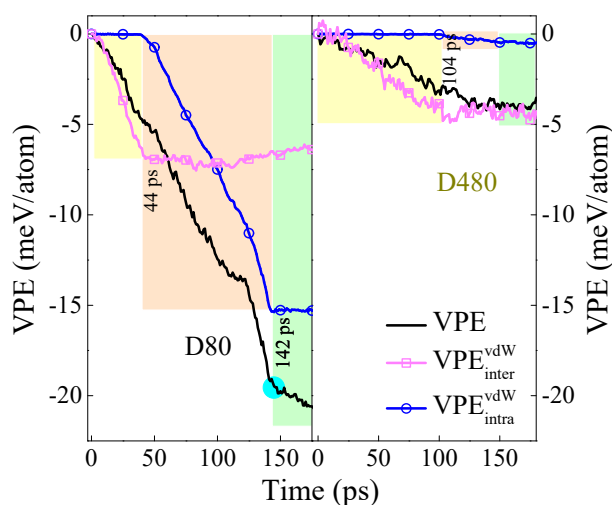

Fig. A.2. Detailed vdW interactions in the systems with gas densities of 80 kg/m³ (denoted as D80) and 480 kg/m³ (D480).
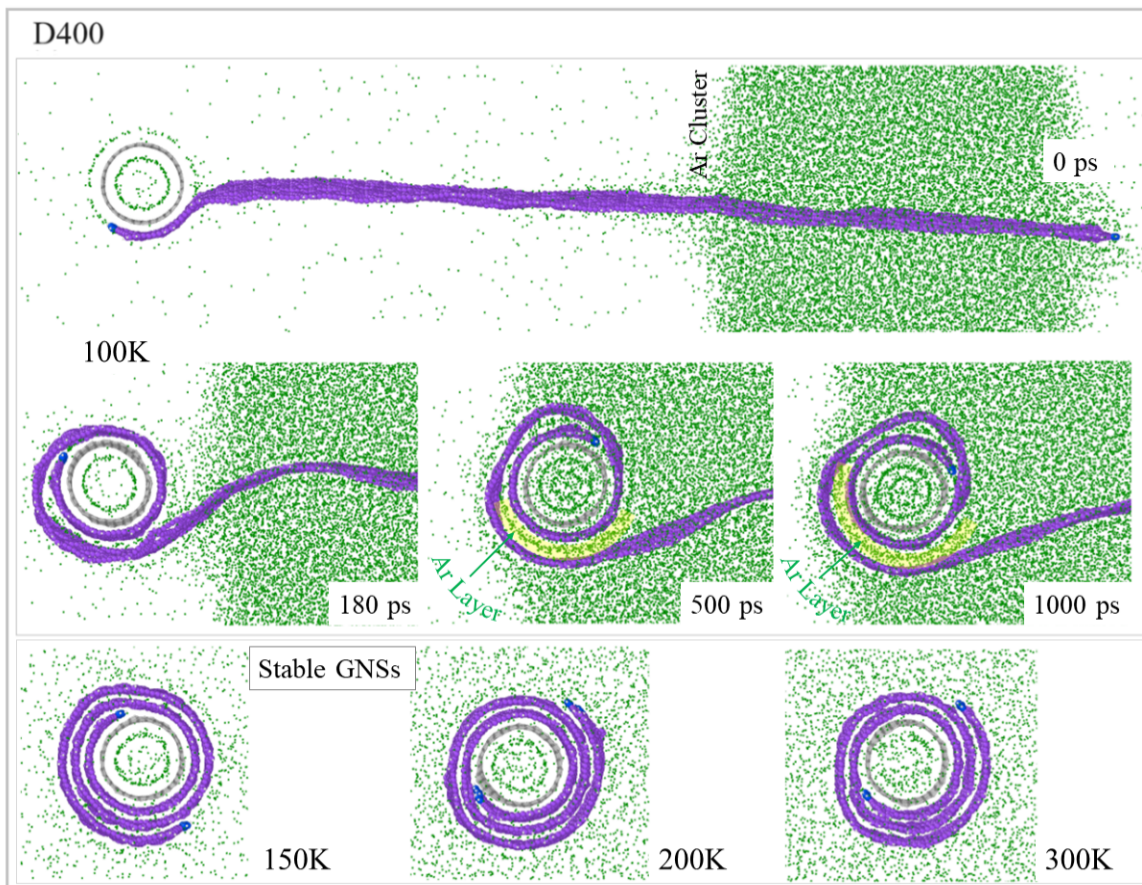
Fig. A.3. Representative snapshots and the final stable configurations of the self-scrolling system in different gas environments at temperatures between 10 K and 300 K with D400.
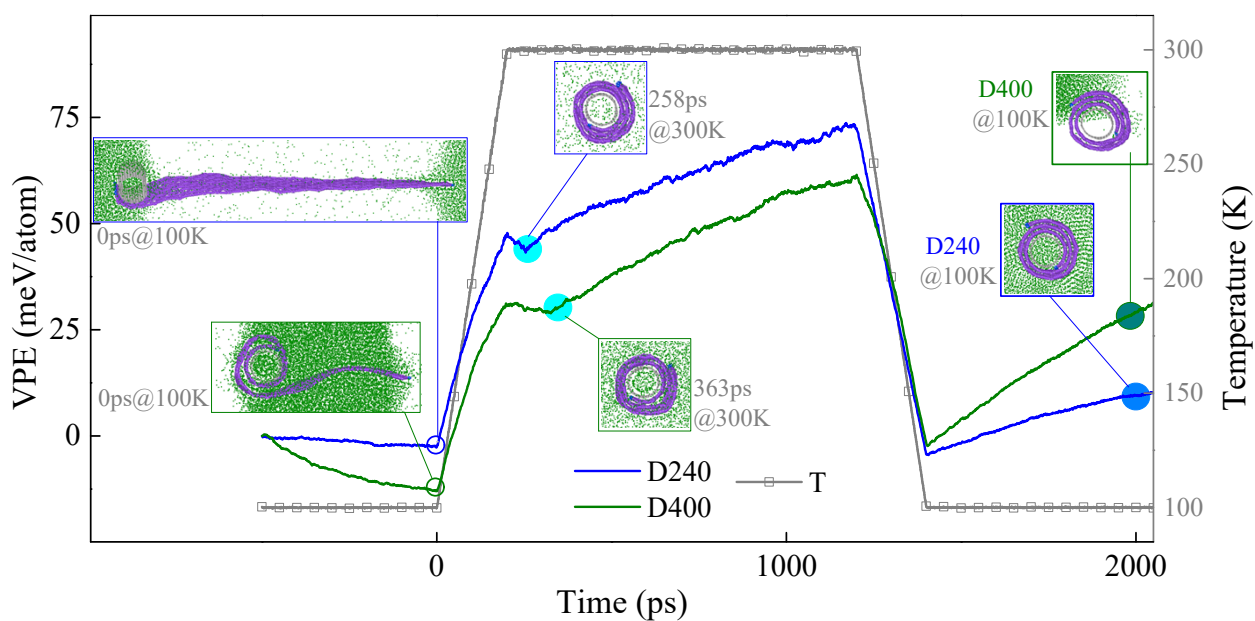

Fig. A.4. VPE per atom of the GNR as well as the system temperature as a function of the simulation time when the system is applied with an annealing treatment varies between 100 K to 300 K.
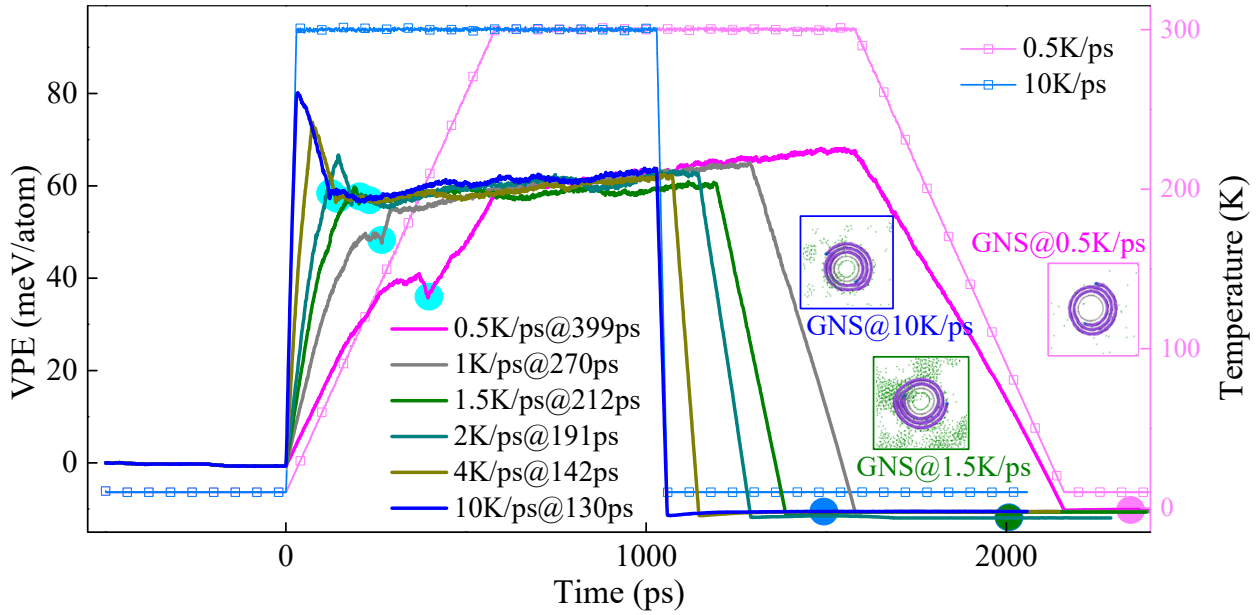
Fig. A.5. VPE per atom of the GNR as well as the system temperature as a function of the simulation time when the system is applied with annealing treatments with different heating/cooling rates varying from 0.5 to 10 K/ps. The temperature varies between 100 K to 300 K. The argon density is 80 kg/m³.
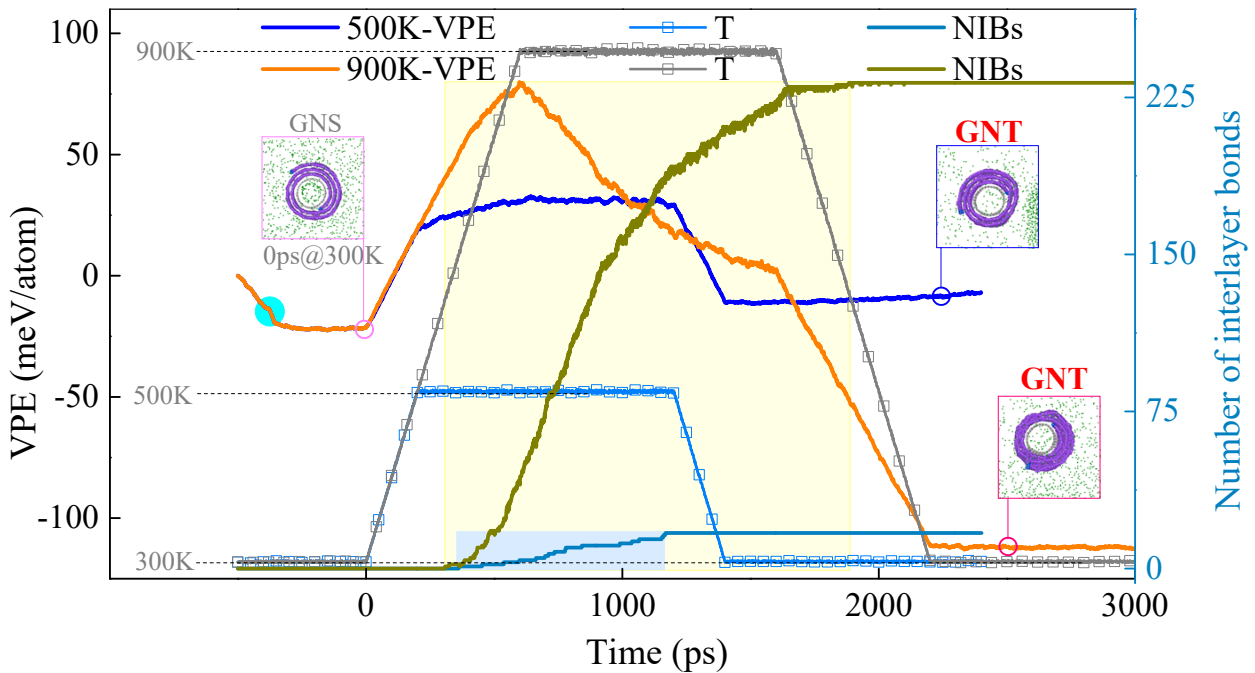

Fig. A.6. VPE per atom of the GNR and the NIBs inside the GNT as a function of the simulation time when the GNR self-scrolling on CNT in argon of D80 with annealing treatments. During the treatment, the heating and cooling rates are fixed at 1 K/ps.