

Supporting Information

Structural and Thermal Stability of Graphyne and Graphdiyne Nanoscroll Structures

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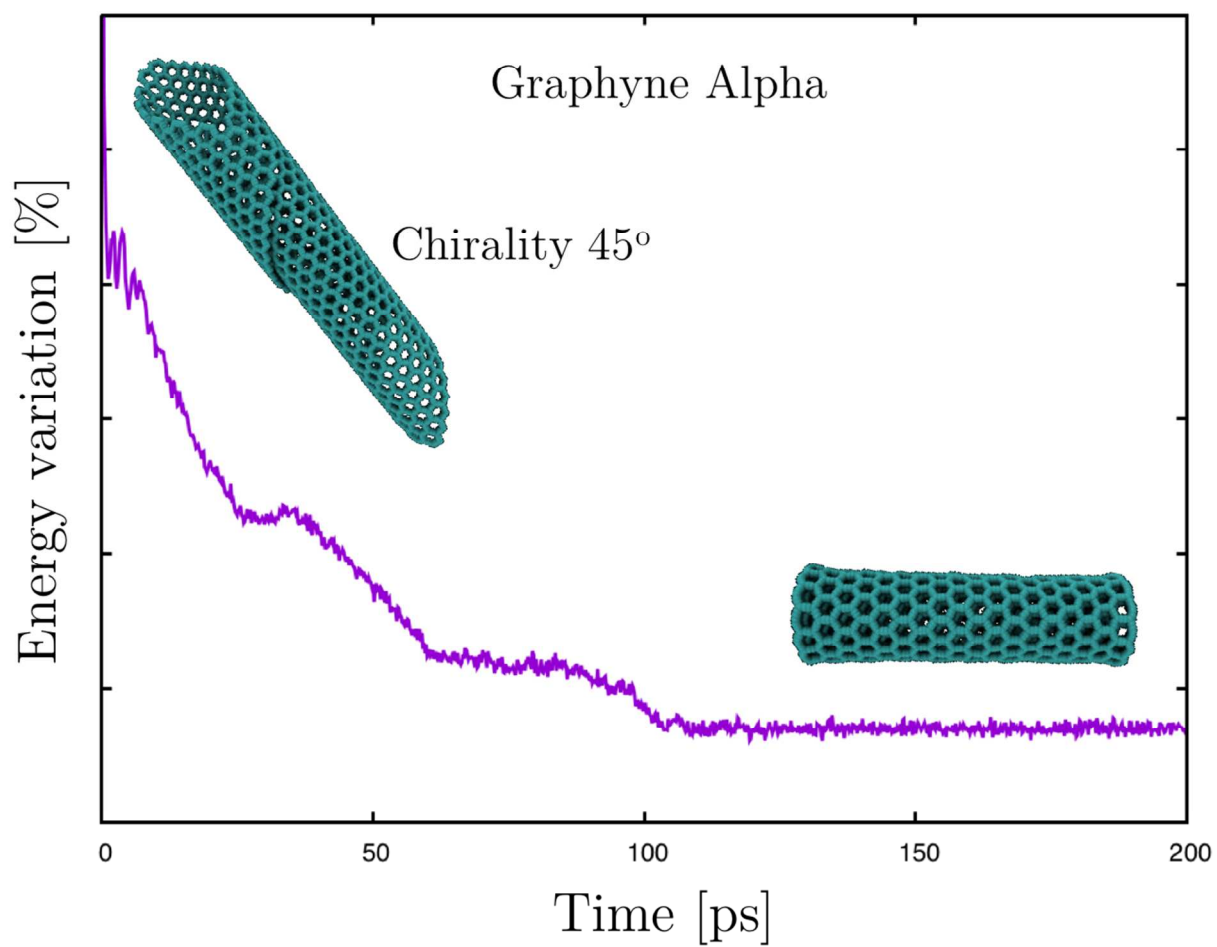


Figure S1 - Energy variation as a function of the simulation time for a chiral graphyne alpha structure with rolling axes 45° . We performed a thermalization at 300K during 200 ps. We can see from the Figure that the chiral structures are not at a minimum energy, thus validating that they are metastable states.

S-2

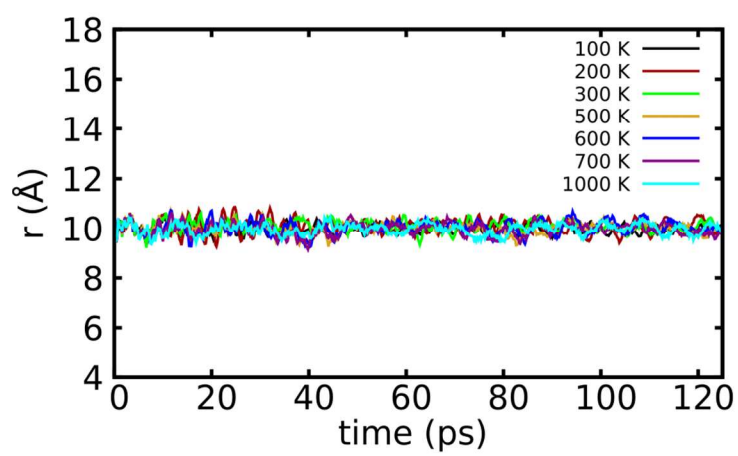


Figure S2 Thermal dependence of graphene nanoscroll inner radius for different temperatures.

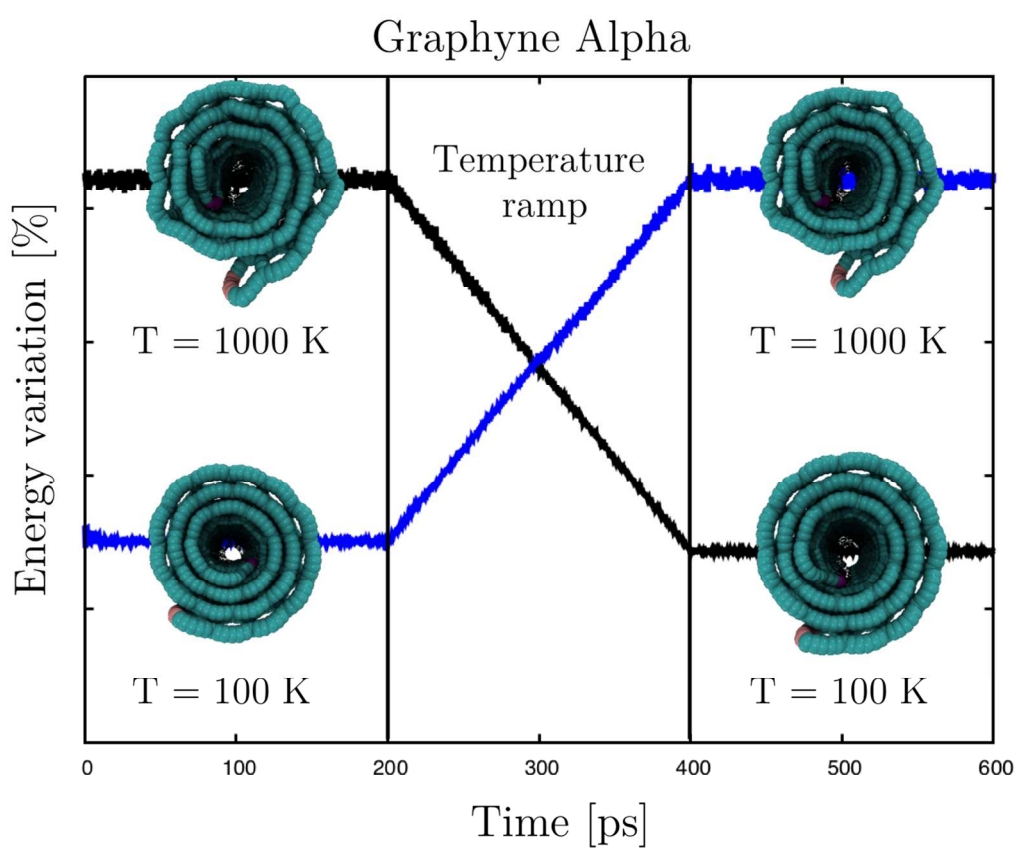


Figure S3. Energy variation as a function of simulation time for heating up (blue) and cooling down (black) for an alpha-graphyne and their corresponding MD snapshots. The heat up and cool down process are thermalized during 200 ps before applying the temperature ramp.

