Supplementary Information for

Nature-inspired Entwined Coiled Carbon Mechanical Metamaterials: Molecular Dynamics Simulations

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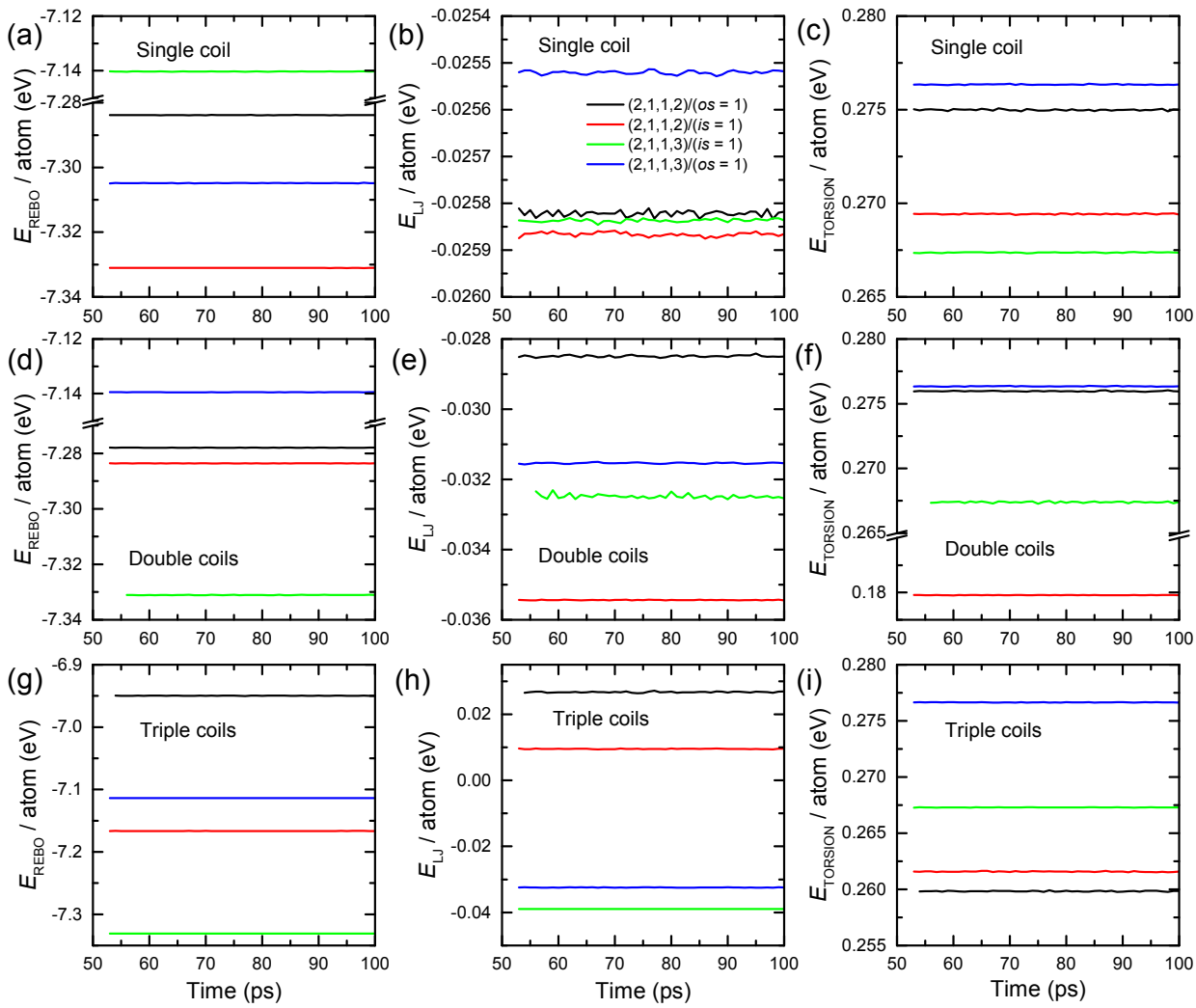

Figure S1 Variations in potential energies of both SHCNCs and ECNCs with MD relaxation time. (a) - (c) Evolution of REBO- , LJ- and Torsion potential energies (E_{REBO}, E_{LJ} and E_{Torsion}) of single-helix. (d) - (f) Development of REBO- , LJ- and Torsion potential energies (E_{REBO}, E_{LJ} and E_{Torsion}) of double-helix. (g) - (i) Changes in REBO- , LJ- and Torsion potential energies (E_{REBO}, E_{LJ} and E_{Torsion}) of triple-helix.

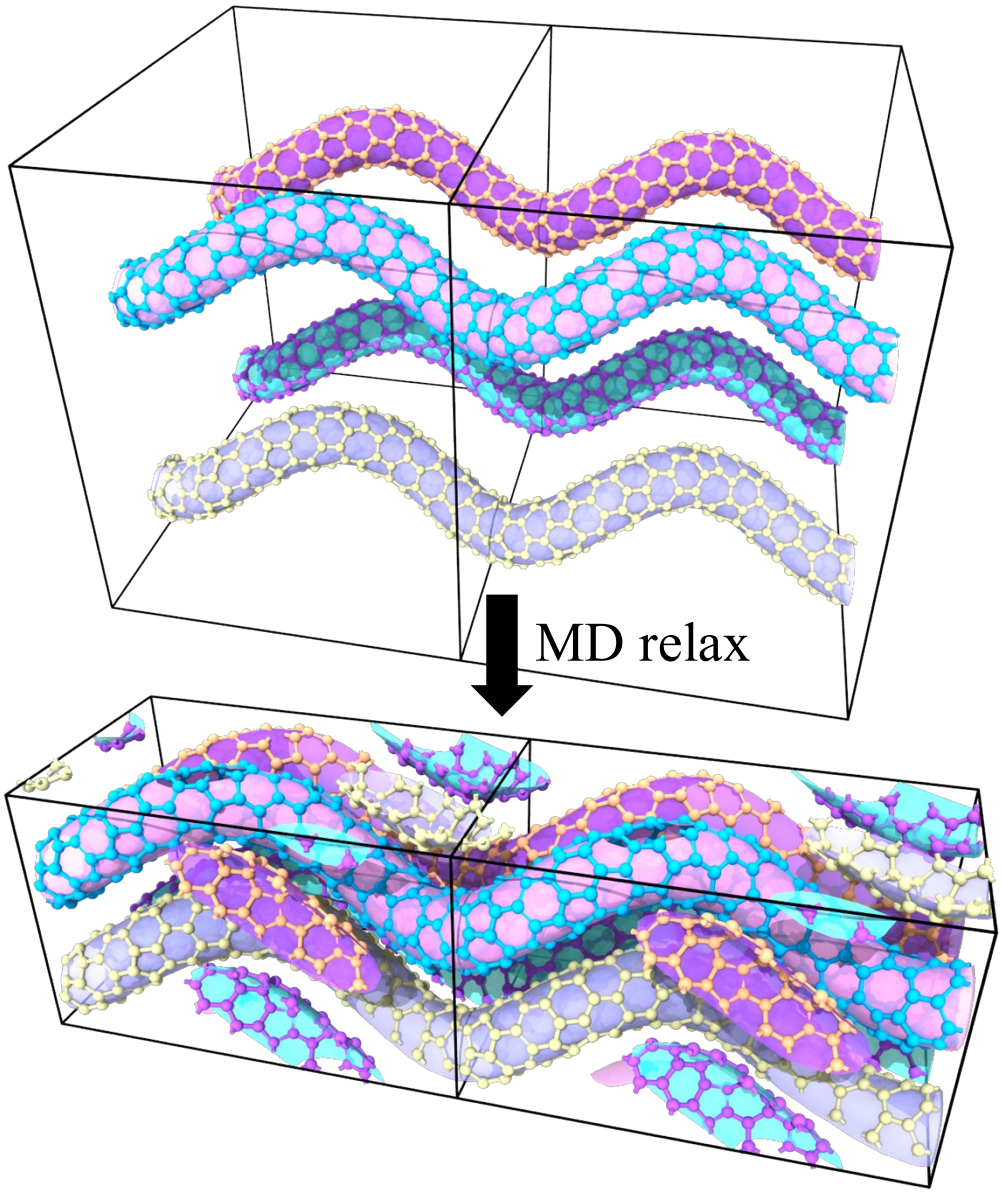

Figure S2 Perspective view of one representative bundle composed of 4-identical carbon nanohelixes with index of (2,1,1,2)/(*os* = 1).

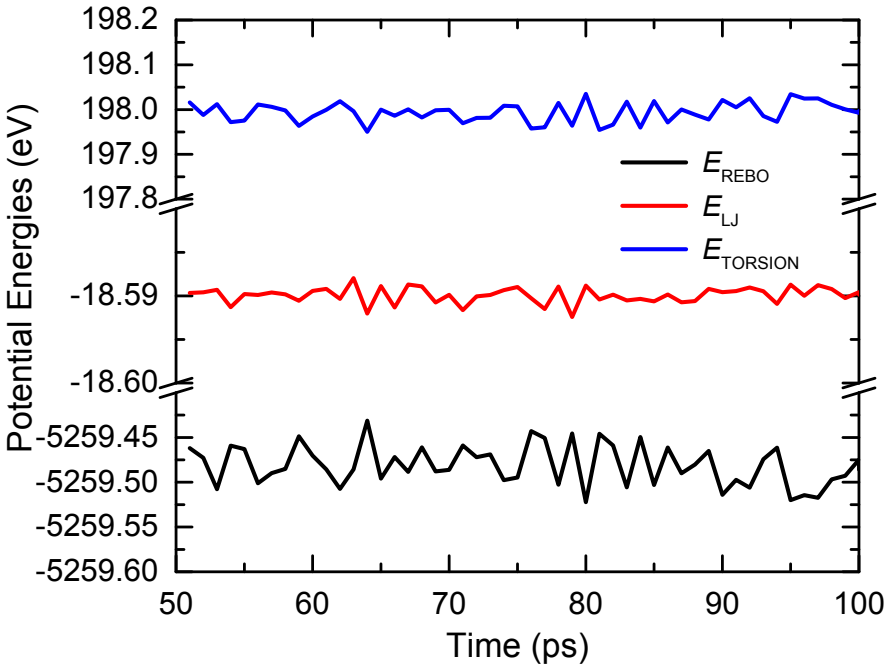

Figure S3 Variation in REBO, LJ and TORSION potential energies with MD relaxation time for entwined-free (2,1,1,2)/(*os* = 1) nanohelix bundle.

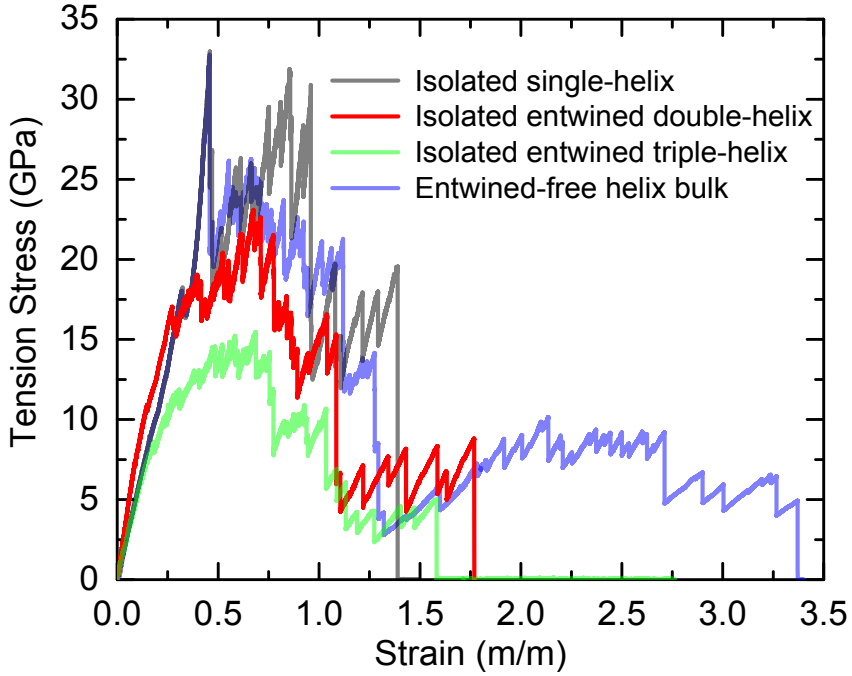

Figure S4 Mechanical tensile stress-strain curves of isolated single-helix, isolated entwined double- and triple-helixes, and entwined-free nanohelix bundle.

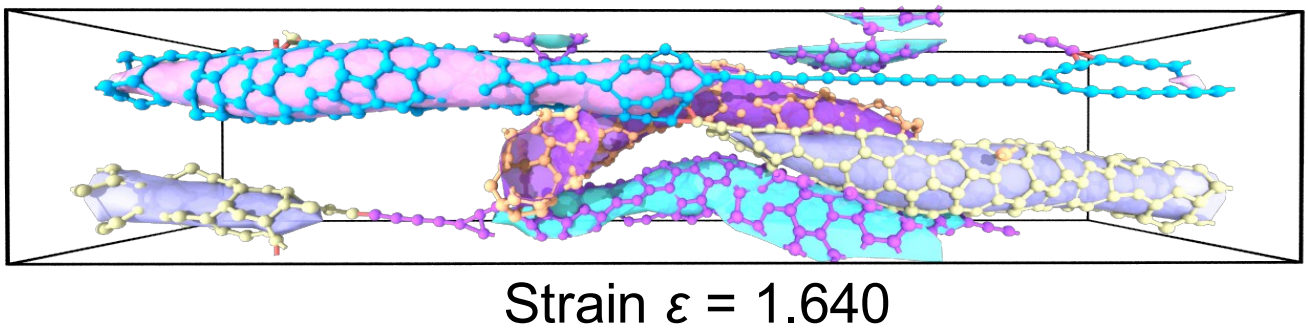

Figure S5 Snapshot of nanohelix bundle at strain of 1.640.