Supplementary Materials

Guide to propose the trial atomic fluctuations of the internal carbyne at each MCS [19]

- The trial fluctuations (δx, δy, δz) of the randomly selected carbon atom along x, y and z axis:

  $\delta x = \pm v < \delta t > R_c$

  $\delta y = \delta z \sim \frac{k_B T}{< E_1 + E_2 + E_3 >} \delta x$

  The free particle velocity is $v = \sqrt{\frac{k_B T}{M}}$.

  The average scattering time $< \delta t > \sim 10^{-13}$s

  M: The mass of a carbon atom.

  R_c: Random number within 0 and 1

  k_B: Boltzmann constant

  $< E_1 + E_2 + E_3 >$: The average energy of single, double and triple bond.

- The stable carbyne chain inside the host should have a shorter mean free path (MFP) and a narrower range of spatial fluctuation compared to an unstable isolated carbyne chain. Hence, the Hooke's factor $f(Hooke)$ is created to refine the trial atomic fluctuation.

  $$f(Hooke) = \frac{K_{break}\left(l_{\max} - < l_{eq} >\right)}{K_{carbyne@host}\left(l_{carbyne@host}\big|_{0K} - < l_{eq} >\right)}$$

  The refined trial dynamics (δx', δy', δz') = ($\delta x \cdot f(Hooke)$, $\delta y \cdot f(Hooke)$, $\delta z \cdot f(Hooke)$) monitoring from a chain-breaking state to a crystalline form.

  Chain-breakage: the maximum $C-C$ length = $l_{\max} \sim 1.73$ Å associated with the spring constant K_{break}.

  The ground state of an isolated LCC: bond length = $< l_{eq} > \sim 1.34$Å

The average bond length of the internal LCC in the host at 0K = $l_{carbyne@host}\big|_{0K}$ associated with the spring constant $K_{carbyne@host}$.

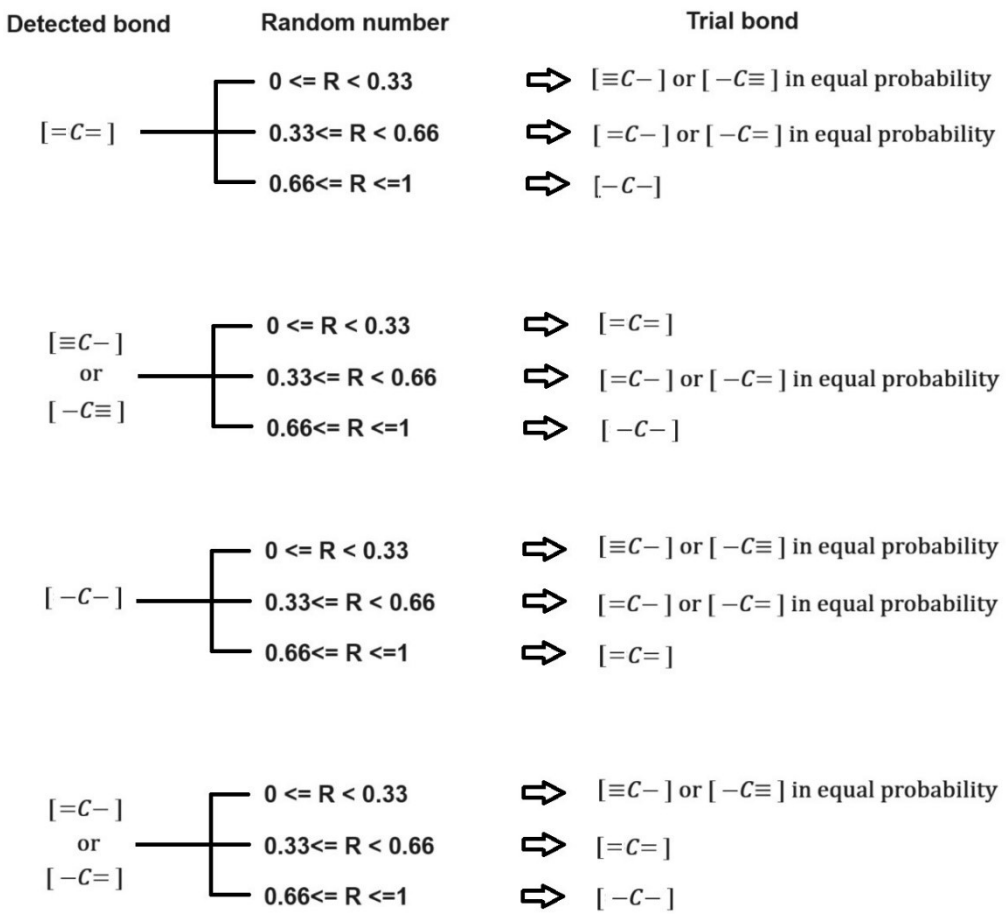

Figure S1: Guide to propose the trial type of covalent bond of the internal carbyne at each MCS [19]