CATALYTIC SYNTHESIS KINETICS OF ENDOHEDRAL GNRS

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Understanding the growth mechanisms of graphene nanoribbons (GNRs), particularly for chirality-controlled synthesis, remains a challenge. This study investigates the atomic-level synthesis of endohedral GNRs (with encapsulated Ni catalyst) using reactive molecular dynamics simulations with acetone, methanol, acetic acid, and dimethyl ether. Similar to catalytic single-walled carbon nanotube (SWNT) growth [1], the numbers of defective and defect-free rings dynamically change. Defect-free rings form preferentially, leading to predominantly defect-free structures (Fig. 1a). The total number of rings varies with precursor gas (Fig. 1b), with methanol yielding the highest and acetone the lowest, likely due to reactivity differences. These findings offer insights into endohedral GNR growth, informing controlled synthesis strategies.

**Figure 1** (*a*) Number of defective and defect-free rings as a function of time (acetic acid); (*b*) GNR ring formation rate for different precursor gases.

REFERENCES

[1] U. Khalilov et al., Nanoscale Horizons **4**, 674 (2019).