CANDIDATE FOR SYNTHESIZING ENDOHEDRAL GRAPHENE NANORIBBON WITH PRECISE CHIRALITY

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While current research enables the synthesis of graphene nanoribbons (GNRs) within single-walled carbon nanotubes (SWNTs) [1], achieving the synthesis of GNRs with precise chirality remains challenging. In this regard, we investigate the catalytic synthesis of endohedral GNRs from various hydrocarbon molecules using molecular dynamics simulations. A nickel cluster is introduced as a catalyst in the (10,10) tube. Preliminary results indicate the possibility of synthesizing a precise edge structure (e.g., 4-ZGNR) using the acetic acid (CH3COOH) precursor (Fig. 1*a*). Specifically, after saturating the catalyst nanoparticle with dissolved carbon atoms, adsorbed and dissociated molecules/atoms contribute to the formation of incipient carbon nanostructures (Fig. 1*b*), similar to catalytic SWNT nucleation [2].

Fig.1 *a*) Growth process of GNR from acetic acid molecule. Here, Ni, C, O and H atoms in green, grey, red and blue colors, respectively. b) Distribution of adsorbed C atoms to the concentration of catalyst C atoms (pink) and ring-related C atoms (blue) during the growth of GNR.

REFERENCES

1. U. Khalilov et al., Carbon 2021, **171**, 72.

2. U. Khalilov et al., Nanoscale Horizons 2019, **4**, 674.