Electronic Supplementary Material (ESI) for RSC Advances.

Supplementary Information

Nanocatalyst shape and composition during nucleation of single-walled carbon nanotubes

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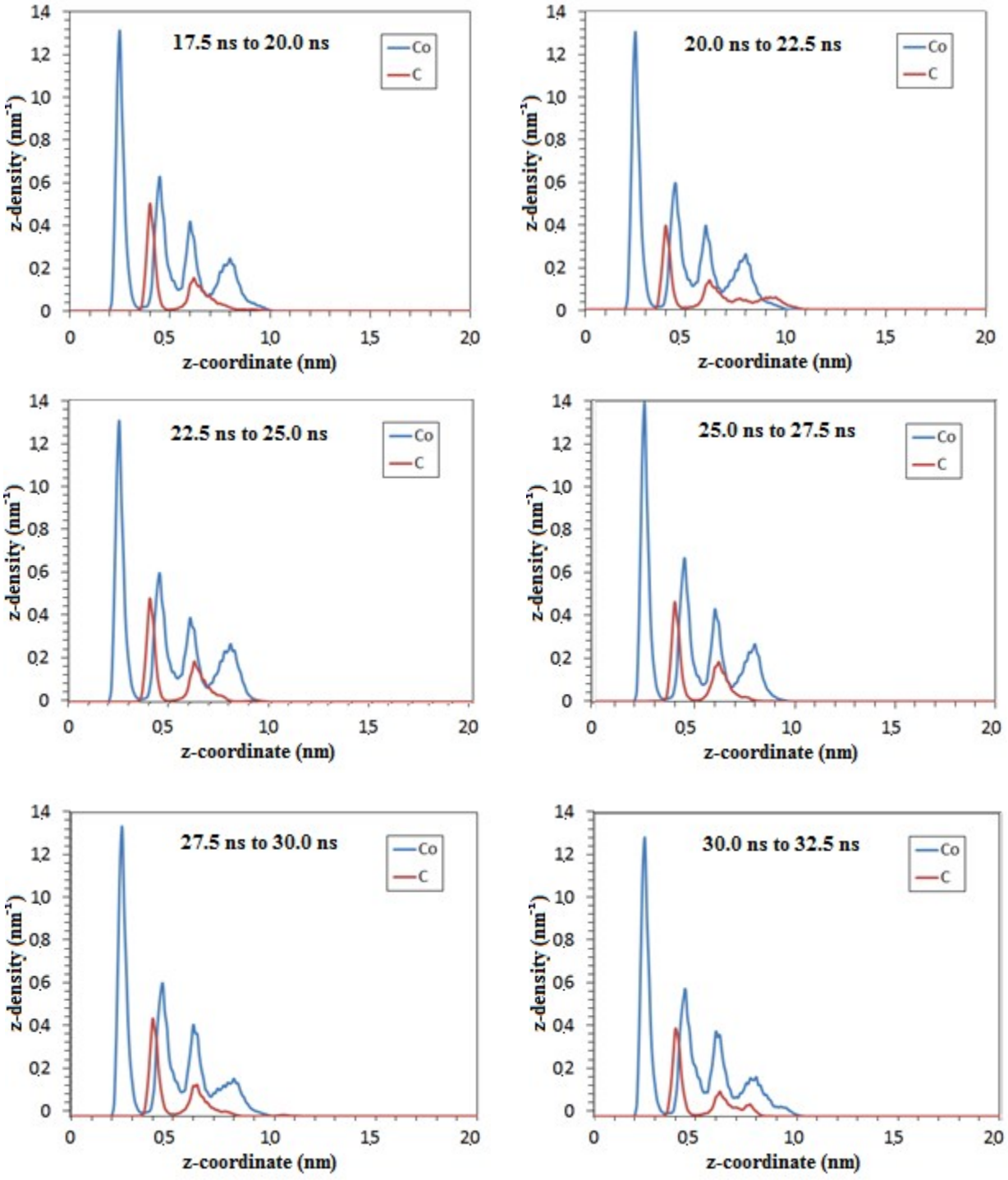

Figure S1. Z-density profiles for cobalt and carbon atoms at different time intervals during the nucleation stage.

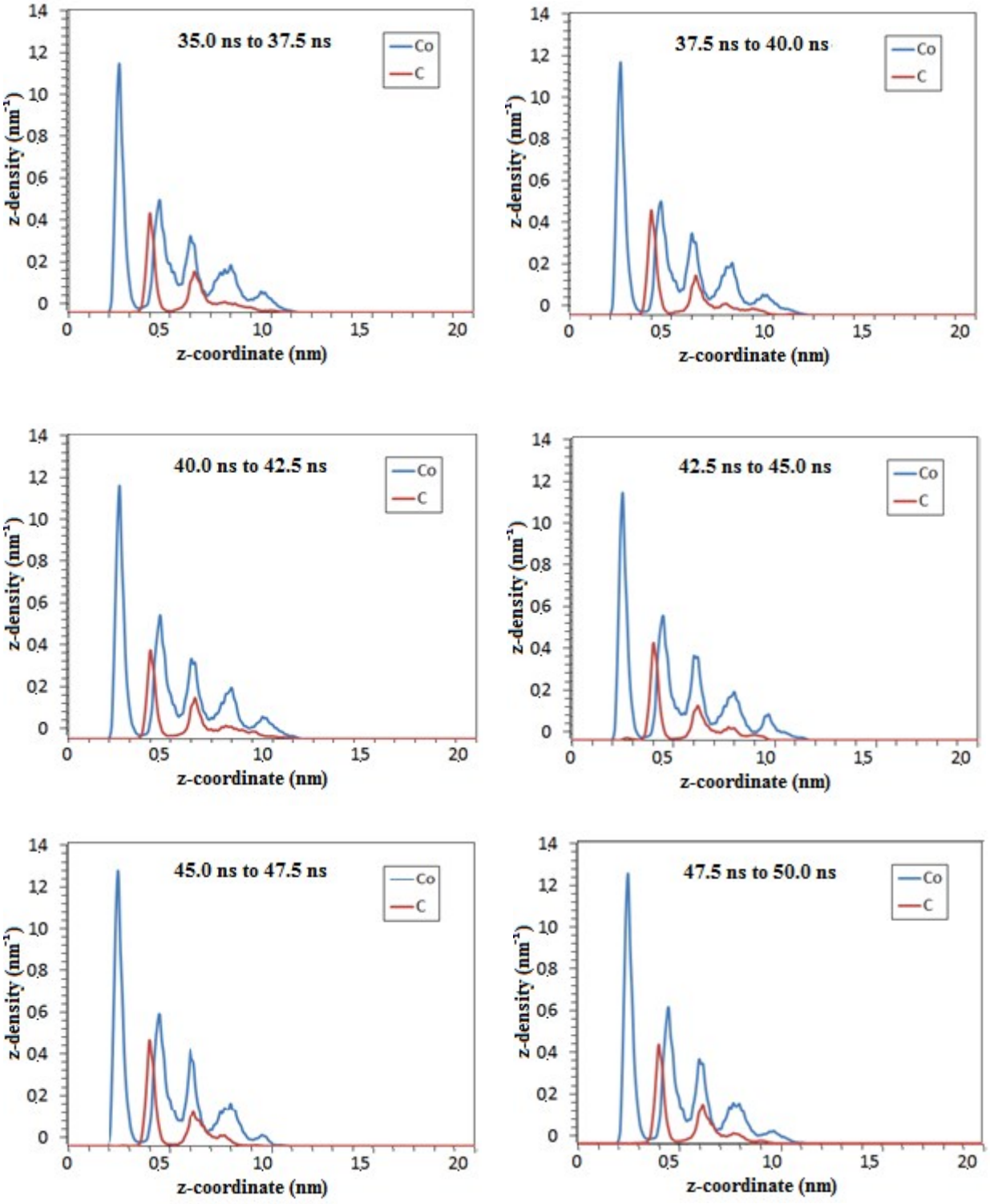

Figure S2. Z-density profiles for cobalt and carbon atoms at different time intervals during the growth stage.

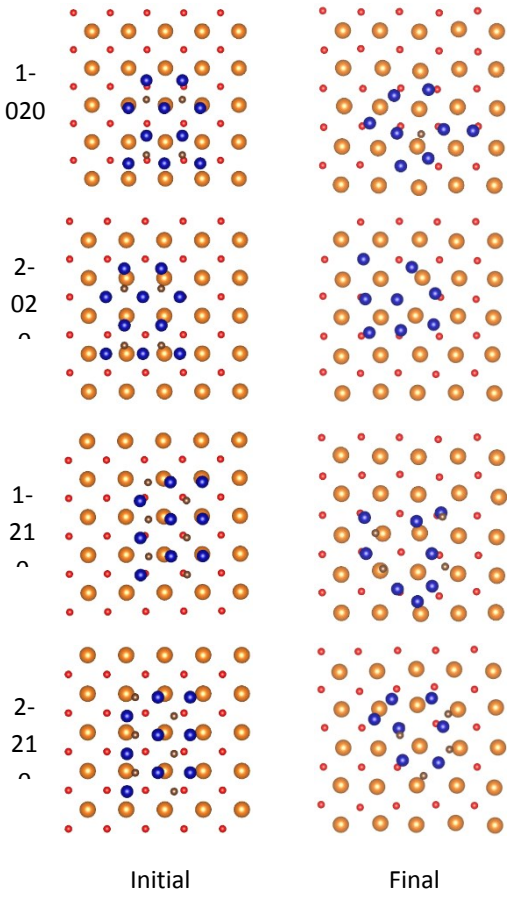

Figure S3. Top view of the first layer of atoms in Co_2C placed in contact with the MgO substrate in the initial configuration (left) and final configuration after 3 ps of ab initio molecular dynamics simulations (right). Each of the surface facets ({020} and {210}) considered for the Co_2C nanoparticle model was initially placed on the MgO surface to either maximize (cases labelled as 1-020 and 1-210) or minimize (cases labelled as 2-020 and 2-210) the number of Co atoms directly on top of Mg atoms. Co atoms in final configuration prefer to be located atop O atoms.

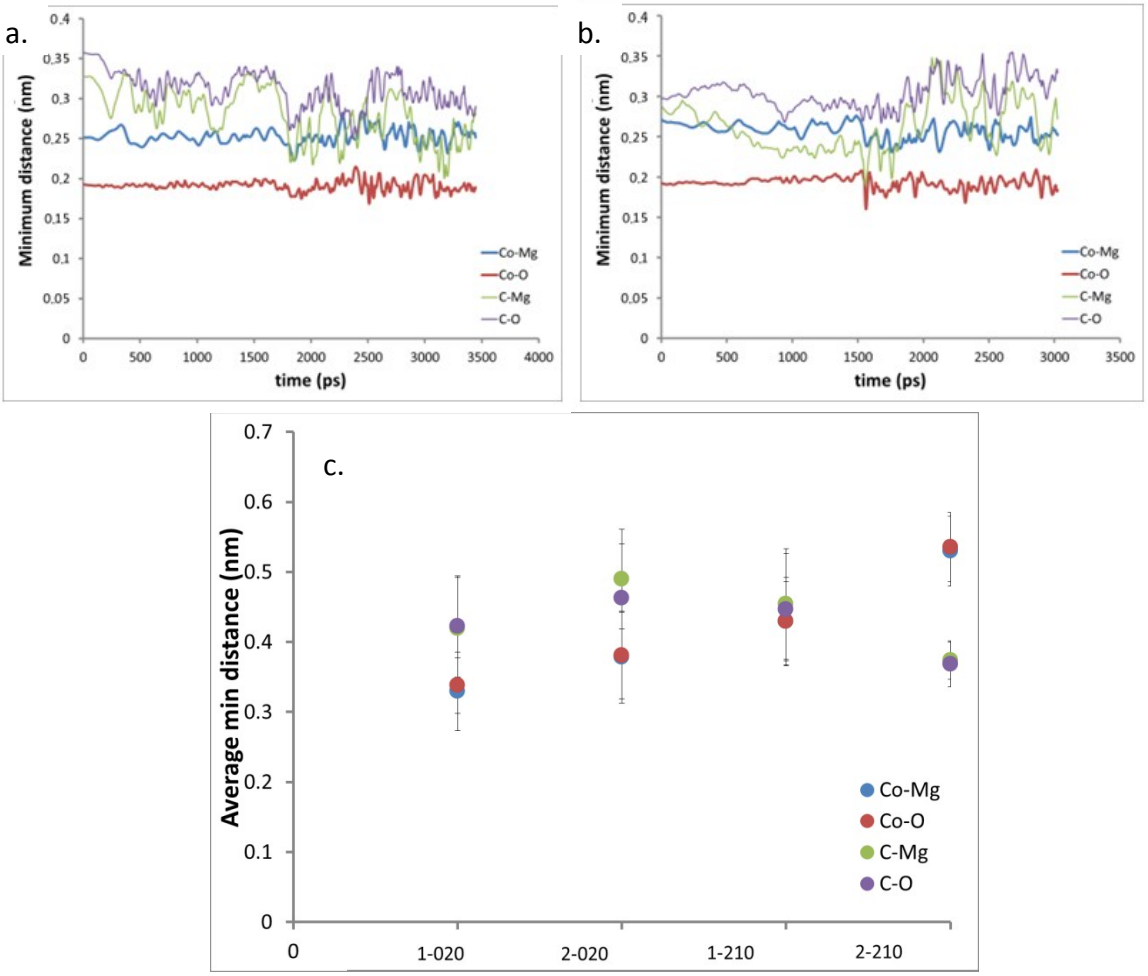

Figure S4. Minimum distances between atom pairs in the nanoparticle and substrate (Co-Mg, Co-O, C-Mg and C-O). Two cases are shown for illustration: a. 1-020 and b. 1-210. The average closest distance between atom pairs is shown in numeral c. A greater separation between the Co and C distances relative to the substrate in a. compared to b. reflects features of the initial configuration with the nanoparticle bottom layer containing Co atoms only in the former case and both Co and C atoms present in the bottom layer of the latter. The preference of Co atoms to remain closer to O atoms observed in figure S1 is also apparent from the average minimum distance between atom pairs shown in numeral c. C-Mg and Co-Mg minimum distances are almost identical and C-O distances are slightly bigger and uniform across configurations, however C atoms relative arrangement seem not to be influenced by the substrate. Thus, inference about the evolution of the composition of the nanoparticle layer in contact with the substrate indicates that almost only Co atoms atop O atoms tend to be located at the interface and subsequent layers contain both C and Co atoms (Figure S3).

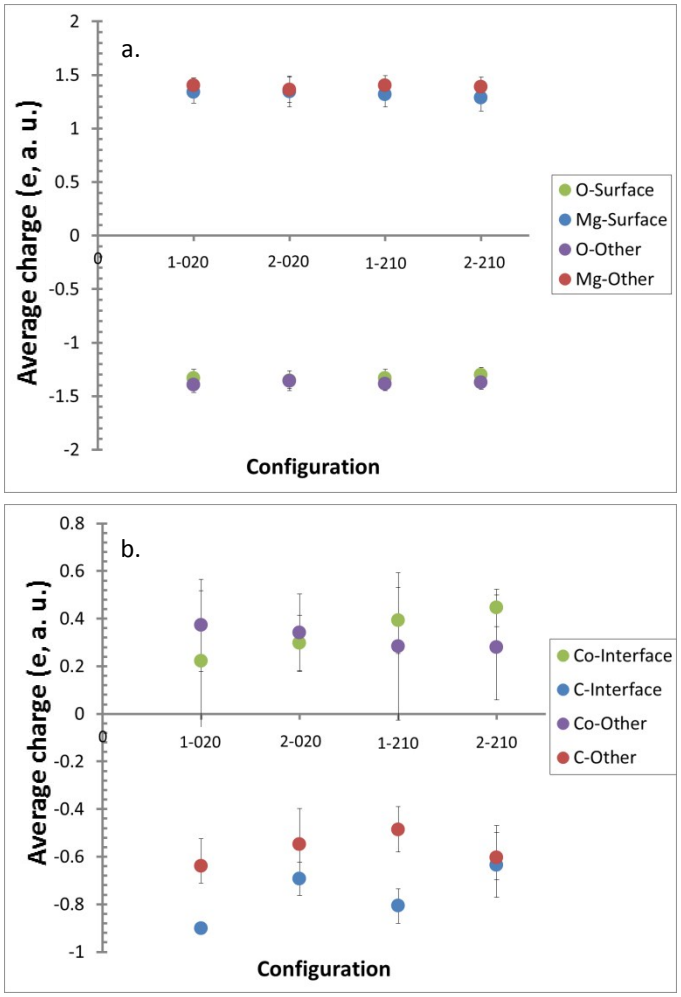

Figure S5. Average atomic charges calculated using the Bader analysis of charges. Atomic charges for the substrate atoms are shown in the top panel and nanoparticle atoms in the bottom panel. A distinction between atoms located near the interface and those located elsewhere is made. Charge magnitudes of Mg and O are symmetrical and uniform across model systems. No significant difference is found between surface and inner-layer atoms in the substrate. C atoms located closer to the interface tend to be slightly more polarized than Co atoms and other C atoms in all cases; on the other hand interfacial Co atoms are more weakly charged than other Co atoms for the (020) cases, whereas the opposite is observed for the (210) cases.