## **Title**

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Main text. Please make your words not more than 1500 and do not use images as far as possible. [1] Reference 1. [2] Reference 2.

Two samples on next page may help you:

## Origination of chirality selectivity in single-walled carbon nanotube growth catalyzed by tungsten-based intermetallic compounds: a theoretical study

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Synthesis of single-walled carbon nanotubes (SWNTs) with identical specific chirality is the paramount objective in the catalytic chemical vapor deposition (CCVD) method. Using tungsten-based intermetallic compounds as catalysts, we have achieved unprecedented high selectivity towards SWNTs with specific chiralities[1]. In this study, there are experimental evidences showing that the unique structure of the catalyst may act as the structural template for SWNT. Then we systematically studied the structural match between SWNTs and different catalysts with first-principles calculations. The structural match energy variations in the tungsten-based intermetallic compounds are universally higher than those in the corresponding monometallic catalysts, implying a higher specific selectivity towards certain chiralities. Anisotropic structures of the tungsten-based intermetallic compounds, i. e. lower symmetry and unique atomic arrangements are key factors for their high single-chirality selectivity towards SWNTs.

[1] F. Yang, X. Wang, D. Zhang, J. Yang, Y. Li\* et al., Nature 2014, 510, 522-524.

## Synthesis and characterization of SWNTs using W-Co catalyst with low pressure CVD

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Chirality controlled growth of SWNTs is highly expected toward the applications of SWNTs. Recently, it was reported that  $W_6\mathrm{Co_7}$  alloy catalyst realized the growth of single-chirality SWNTs with purity over 90 % through pretreatment and growth at high temperature [1]. In order to investigate the controlled-growth mechanism and to conduct the experiment safely, we grew SWNTs using W-Co catalyst via ethanol CVD under much less hydrogen and lower pressure conditions. Owing to a narrow growth window of SWNTs at high temperature, we varied the growth parameters to search for appropriate conditions. We changed reduction temperature (800-1030 C), reduction time (3-10 min.), synthesis temperature (800-1030 C), synthesis time (10-20 min.), partial pressure of ethanol (100-1300 Pa), partial pressure of hydrogen by  $\mathrm{Ar/H_2}$  gas (0-150 Pa), and so on. As a result, we succeeded in growing SWNTs at over 1000 C under a condition where partial pressure of ethanol and hydrogen was 100 and 150 Pa, respectively, and total pressure was 5.0 kPa. Raman spectra of the grown SWNTs were measured to examine the chirality distribution. [1] F. Yang et al., Nature 510, 522 (2014).