

## Electronic Supplementary Information

### Key Roles of Carbon Solubility in Single-Walled Carbon Nanotube Nucleation and Growth

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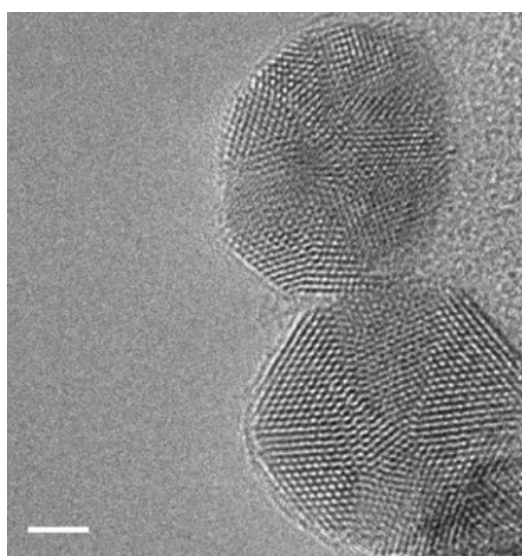
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## More details for **Calculation Methods**

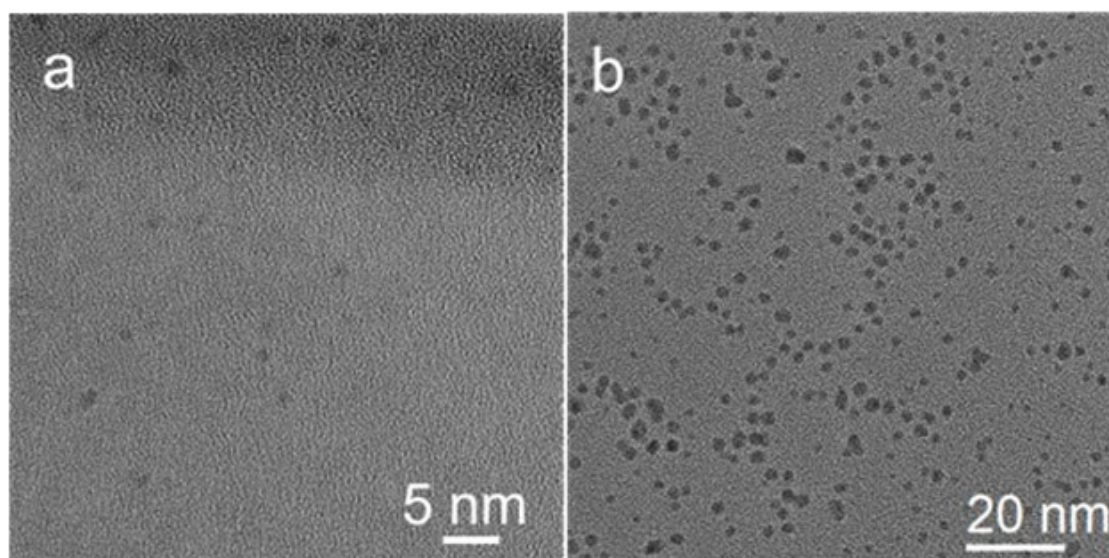
In our TB model a minimal basis, included  $s$  and  $p$  electrons of carbon and  $d$  electrons of Ni, is required to obtain a transferable TB model of the C-C, Ni-Ni, and Ni-C interactions applicable to binary systems.<sup>1</sup> We first assume the same atomic energy levels for carbon proposed by Xu *et al.*<sup>2</sup> ( $\epsilon_s = -2.99$  eV and  $\epsilon_p = 3.71$  eV) and second, to reproduce energetic properties of transition metal carbides it is reasonable to fix the relative position of  $p$  and  $d$  atomic energy levels accordingly. For NiC, this leads to  $\epsilon_d = -0.5$  eV. In the case of noble elements,  $s$  and  $p$  states of the metallic element should be kept. When interested in detailed electronic structure properties,  $sp-d$  hybridization should however be taken into account and this can be done, as shown, for example by Barreteau *et al.*<sup>3</sup> Since we are interested in cohesive energies more than in a detailed description of the electronic structure, we have chosen to use the simplest basis where the contribution of these states is neglected. With the same framework, we take advantage of the physical transparency of the model to validate the influence of some key parameters on carbon solubility. To illustrate this particular point, let us now discuss the electronic structure of typical NaCl-type carbide. In this case, the shape of the hybridized band does not change too much when varying the element of the transition series.<sup>1</sup> The binding contribution is mainly due to the  $pd$  hybridization between the  $p$  states of carbon and the  $d$  states of the metallic element.

## **References** for Supplementary Information:

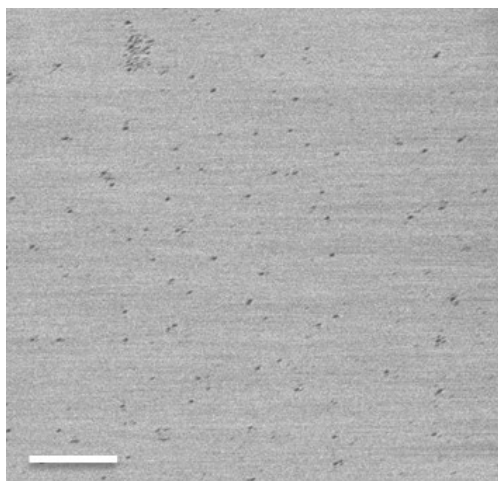
1. H. Amara, F. Ducastelle, J.-M. Roussel, C. Bichara, J.-P. Gaspard, *Phys. Rev. B* 2009, **79**, 014109.
2. C. H. Xu, C. Z. Wang, C. T. Chan, H. K. M., *J. Phys.: Condens. Matter* 1992, **4**, 6047.
3. C. Barreteau, R. Guirado-López, D. Spanjaard, M. C. Desjonqueres, A. M. Oleś, *Phys. Rev. B* 2000, **61**, 7781.



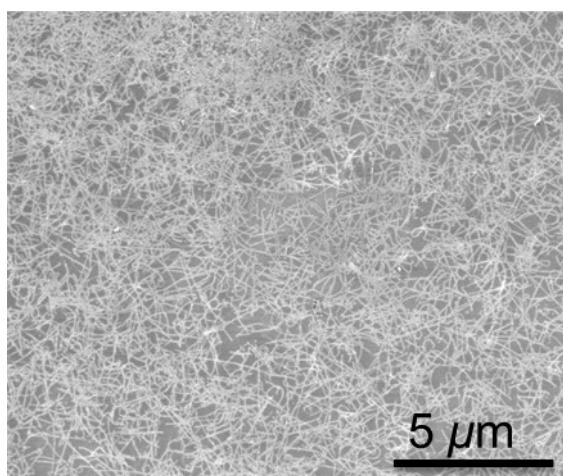
**Figure S1** High resolution TEM image of as-received Au nanoparticles, showing that Au nanoparticles adopt icosahedral structure. Scale bar is 2 nm.



**Figure S2** TEM images of Au nanoparticles with diameters of (a) 1.4 nm and (b) 3.0 nm.



**Figure S3** SEM image of 450 °C-annealed Au NPs after subjected to ambient CO CVD growth at 800 °C for 1h. Scale bar in the image is 1  $\mu\text{m}$ .



**Figure S4** SEM image of 800 °C-annealed Au NPs (1.4 nm) after subjected to ambient CO CVD growth at 800 °C for 1h.