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Molecular dynamics study of catalytic ability of transition metals in nucleation process of SWNTs

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Interaction between catalytic metals and carbon atoms on formation process of SWNTs are studied by the home-made multi-body potentials base on density functional theory calculations of small metal-carbon binary clusters. The Co cluster has a partially crystal structure where metal atoms are regularly allocated and embedded in the hexagonal carbon network. On the other hand, carbon atoms cover the entire surface of the Fe cluster. The number of hexagonal rings in the Co cluster increase about two times faster than in the Fe cluster. This implies stronger interaction between the graphitic lattice and Co atoms than Fe atoms. The difference of graphitization ability may reflect the ability as a catalyst on the formation process of SWNTs.

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