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The possibility of high-performance n-type carbon nanotube devices by fullerene functionalization: A first-principles study¹ YONG-HOON KIM, University of Seoul, GA IN LEE, JEUNGKU KANG, Korea Advanced Institute of Science and Technology — The successive appearance of low-dimensional carbon nanomaterials, such as zero-dimensional [60]fullerene (C60), one-dimensional carbon nanotube (CNT), and two-dimensional graphene, has been an inexhaustible source for the study of novel scientific principles and the search of advanced technological applications. Recently, about a decade after the discovery of the first C60-CNT hybrid form, carbon nanopeapod, a new hybrid C60-CNT nanostructure termed as “carbon nanobud” has been synthesized [1]. Extending our earlier study of polymerized C60 nanowires [2], we here apply a first-principles computational approach [3] to consider the C60 functionalization of CNTs as a scheme to engineer the CNT-metal contacts to produce reliable high-performance n-type CNT devices. References: [1] A.G. Nasibulin, et al., *Nat. Nanotechnol.* 2, 156 (2007). [2] G. I. Lee, J. K. Kang, and Y.-H. Kim, *J. Phys. Chem. C* 112, 7029 (2008). [3] Y.-H. Kim et al., *Phys. Rev. Lett.* 94, 156801 (2005).

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Yong-Hoon Kim
University of Seoul

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