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Charge injection and transport across metal-C60 and C60-petacene interfaces: A first-principles study[1] YONG-HOON KIM, Korea Advanced Institute of Science and Technology — Recent experiments demonstrated that [60]fullerene (C_{60}) molecules adsorbed on metal surfaces provide favorable energy level alignment for both electron and hole injections in the context of light-emitting diode applications [1,2]. The efficient hole injection across C_{60} layers is rather surprising, since C_{60}s are highly electron-accepting molecules and should behave as a hole blocking (rather than hole injection) layer. To provide a microscopic understanding of these seemingly contradictory finding, we consider Au–C_{60}–pentacene–C_{60}–Au molecular junctions using a first-principles computational approach. We find the Fermi level pinning at the Au–C_{60} interfaces and the strongly configuration-dependent charge transport efficiency at the C_{60}–pentacene interfaces. The former finding is in agreement with a recent experimental report [2] and our earlier conclusion from the study of polymerized C_{60} wires [3]. We will explain the latter observation based on the nature of charge tunneling across π–π orbitals [1] Lee, J.Y., Appl. Phys. Lett. **88**, 073512 (2006) [2] Wang, Z.B *et al.*, Appl. Phys. Lett. **95**, 043302 (2009). [3] Lee, G.I., Kang, J.K., & Kim, Y.-H., J. Phys. Chem. C **112**, 7029 (2008).

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