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First-principles study of charge injection and transport through pentacene multilayers[1] YONG-HOON KIM, University of Seoul — Applying a combined density-functional theory and matrix-Green's function approach [1,2], I study the coherent charge transport properties of pentacene nanowires sandwiched between Au(111) electrodes. Junction models based on pentacene trilayers in the ideal π-stacked and herringbone arrangements with the face-on and edge-on contact configurations at different contact distances are considered. I show that pentacene wires exhibit a robust p-type conductance behavior in agreement with experiments, and analyze the physical origin in terms of charge transfer between molecules and metal electrodes.

[1] Y.-H. Kim, S. S. Jang, Y. H. Jang, W. A. Goddard III, Phys. Rev. Lett. **94**, 156801 (2005).
[2] Y.-H. Kim, J. Tahir-Kheli, P. A. Schultz, and W. A. Goddard III, Phys. Rev. B **73**, 235419 (2006).

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