Opportunities for Single-Molecule Electronics: A Ten-Year Perspective

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Molecular electronics is a rapid developing discipline since the end of the 20th century as an important subject arising out of nanoelectronics and other emerging fields, with the aim to investigate, regulate and exploit the charge transport properties of a single molecule, cluster, supramolecule and corresponding functional assembly [1]. It also focuses the scientific interdisciplinary issues from physics, chemistry, material science and electronic engineering at the nano and even single-molecule scale, for example, the novel photonic, thermal, electric and magnetic phenomena generated through the quantum effect induced by size limit; the characterization of electronic and phononic wavelet functions in nanosystems and their coupling interactions; the quantum tunneling and electronic spin conformation of nanosystems [2,3].

Towards the "More Moore". The original goal of molecular electronics is to build functional molecules from atomic level, and then to build electronic devices and circuits from the individual molecules. One of the major driving forces for molecular electronics aims to assemble logic circuits with a single molecule as the basic electronic component, thereby improving the intensity of devices integrated on chip and further pushing the "More Moore" roadmap. Individual molecules are the smallest material units with the atomic-level precise structure, which can be realized by mass production. Benefiting from the development of synthetic chemistry, single-molecule transistors have unique advantages on the precise modulation of quantum effects such as interference. The integration of the high-performance single-molecule transistors to develop the "molecular circuits" is a milestone for fundamental science and cutting-edge technology. Towards this goal, novel quantum phenomena such as quantum interference effect in the charge transport through single-molecule junction sheds light on high conductance on/off ratio, which also enables potential higher switching ratio and even lower subthreshold swing than traditional transistors when leads to the single-molecule transistors [4,5]. However, the stability of the transistor as well as the integration of multiple devices on chip remained as a major challenge for the fabrication of “molecular circuits”.

Towards single-molecule physical chemistry and sensing applications. In recent years, we extended the application of single-molecule techniques to the quantitative analysis of the molecular physical-chemical process by counting the number of molecules. Interestingly, we found that the single-molecule technique offers more insights beyond the ensemble techniques such as NMR. In this talk, I will share our recent effort towards quantitative analysis of the reaction rate [6], adsorption free energy [7], isomerization [8], the movement manipulation of molecules[9], and even the assembly of molecules at the scale of single or several molecules, suggesting single-molecule electronics provides a unique opportunity for the ultra-sensitive sensing and characterization applications [10].

Towards molecular thermoelectrics. Advances in the fabrication and thermoelectric measurement technique in the nanoscale system allow for the better understanding in heat dissipation or heat transfer in microscopic system [11]. Previous theoretical studies suggest that the thermoelectric devices with molecular monolayer may offer a high thermal conversion efficiency with $ZT > 4$. To investigate the thermoelectric properties of single-molecule devices, the temperature control unit are incorporated for the STM break junction setup for the measurement of the thermopower of various molecular derivatives by introducing custom fabricated temperature-controlled suspended micro electromechanical system (MEMS) with an integrated serpentine Pt heater. The control of electron and heat transport may offer the chance for the next conceptual thermoelectric devices with high ZT.

In summary, although there is still a long way to make molecular electronic device into application, recent advances of the molecular electronics offer new perspective for the fundamental research and applications of single-molecule electronics, which may lead to the device’s application of single-molecule electronics on the field of sensors and thermoelectric devices in the next ten years.

References:

[1] J. C. Cuevas, E. Scheer, *Molecular electronics: an introduction to theory and experiment*, 1st ed. Singapore, Singapore: World Scientific, **2010**.

[2] T. A. Su, M. Neupane, M. L. Steigerwald, L. Venkataraman, C. Nuckolls, *Nat. Rev. Mater.*, **2016**, *1*, 16002.

[3] D. Xiang, X. Wang, C. Jia, T. Lee, X. Guo, *Chem. Rev.*, **2016**, *116*, 4318.
[4] J. Liu, X. Huang, F. Wang, W. Hong, *Acc. Chem. Res.*, **2019**, *52*, 151.
[5] J. Bai, A. Daaoub, S. Sangtarash, X. Li, Y. Tang, Q. Zou, H. Sadaghi, S. Liu, X. Huang, Z. Tan, J. Liu, Y. Yang, J. Shi, G. Mészáros, W. Chen, C. Lambert, W. Hong, *Nat. Mater.*, **2019**, *18*, 364.
[6] X. Huang, C. Tang, J. Li, L.-C. Chen, J. Zheng, P. Zhang, J. Le, R. Li, X. Li, J. Liu, Y. Yang, J. Shi, Z. Chen, M. Bai, H.-L. Zhang, H. Xia, J. Cheng, Z.-Q. Tian, W. Hong, *Sci. Adv.*, **2019**, *5*, eaaw3072, 2019.
[7] C. Zhan, G. Wang, X.-G. Zhang, Z.-H. Li, J.-Y. Wei, Y. Si, Y. Yang, W. Hong, Z.-Q. Tian, *Angew. Chem. Int. Ed.*, **2019**, *58*, 14534.
[8] C. Tang, T. Tang, Y. Ye, Z. Yan, Z. Chen, L. Chen, L. Zhang, J. Liu, J. Shi, H. Xia, W. Hong, "Identifying the conformational isomers of single-molecule cyclohexane at room temperature," *Chem*, **2020**, *6*, 2770.
[9] C. Zhan, G. Wang, J. Yi, J.-Y. Wei, Z.-H. Li, Z.-B. Chen, J. Shi, Y. Yang, W. Hong, Z.-Q. Tian, *Matter*, **2020**, *3*, 1350.
[10] Y. Hu, X. Zhuang, L. Lin, J. Liu, Z. Yao, Z. Xiao, J. Shi, B. Fang, W. Hong, *ACS Sens.*, **2020**, 10.1021/acssensors.0c02038.
[11] H. Chen, S. Sangtarash, G. Li, M. Gantenbein, W. Cao, A. Alqorashi, J. Liu, C. Zhang, Y. Zhang, L. Chen, Y. Chen, O. Gunnar, H. Sadeghi, M. R. Bryce, C. J. Lambert, W. Hong, *Nanoscale*, **2020**, *12*, 15150.

Biography:

Wenjing Hong received his Ph.D. of Science (summa cum laude) on molecular electronics from University of Bern in 2013 under the supervision of Prof. Thomas Wandlowski. He has been a full professor in chemical engineering at Xiamen University since 2015. His current research is mainly focused on single-molecule electronics, thermoelectrics and relevant instrumental development. He has published over sixty papers as the corresponding author, including *Nat. Mater.*, *Sci. Adv.*, *Chem*, *Matter*, *Nat. Commun.*, *J. Am. Chem. Soc.* and *Angew. Chem. Int. Ed.* Details can be found at Pilab.xmu.edu.cn.