Chapter 2
Motivation—Focusing on Molecular Wires

As envisioned above, the rapidly emerging field of molecular electronics offered major incentives to device design and the use of molecular wires [1, 2]. The key idea of using molecules as wires stems from consumer electronics. Let us consider on a journey taking us inside of electronic devices:

Macroscopic wires, namely ordinary metallic wiring, which pass the electron flow in refrigerators, televisions, stereos, computers, household lightning, etc., measure approximately 1 cm in diameter. Going beyond that first level of wiring much smaller wires (approx. 1 mm in diameter) are found on printed circuit boards as they connect smaller components, e.g. resistors, logic chips, rheostats, etc. The next step takes us inside logic chips, for instance. Here, we will come across wires, 10th of a μm wide, which are used to connect solid-state transistors carved out of silicon only. Connecting thousands of such transistors allows performing logic operations. Considering current technologies, this would be pretty much the end of our journey. Reaching beyond this obliges us to overcome the limits of present semiconductor manufacturing methods. Molecular wires would constitute a potential solution. Recent breakthroughs have produced molecular-scale wires, ranging in length from 1 to 100 nm and width from 0.3 nm on up.

In the commercial technology of 2004, the copper wires in Intel's Pentium®4 logic chip are produced in their newest 300 mm wafer fabrication facility in Ireland, and are 90 nm wide [3]. The use of strained silicon [4] is one of several approaches tested to modify present silicon-based processes to meet the demands of the development roadmap. Now, considering a typical molecular wire, investigated in our lab with a width of 0.4 nm and a length of 2.5 nm, see Fig. 2.1. Compared to the Pentium®4 chip 300 of such molecules, side-by-side, would span the 90 nm metal line.

Furthermore, we can tune the physical properties of such a wire in the same way as we can change the raw material used to make it. Thus, the small size, the synthetic diversity, the efficient synthesis of macroscopic amounts in small

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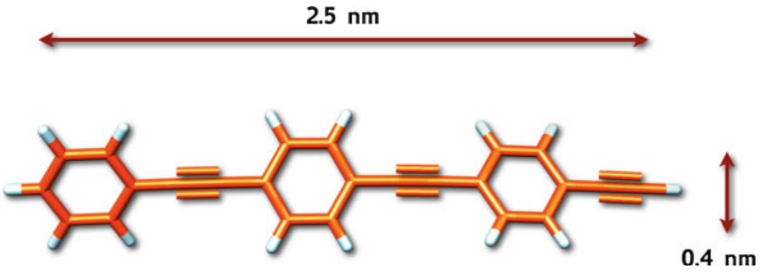

Fig. 2.1 The dimensions of a representative example of a molecular wire are calculated to be 0.4 nm in width and 2.5 nm in length using DFT calculations

reactors are reason enough to prosecute molecular wire research[1] and provide a rational motivation for this thesis: Characterizing several classes of molecular wires.

References

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[1] As an example of how far technology has come, molecular electronics is discussed in the "Emerging Research Devices" section of the most recent International Technology Roadmap for Semiconductors [5] and new molecular wires are a large part of the emerging technology.

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