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Electronics at the molecular level¹

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In the early 1970s, Aviram and Ratner suggested the notion that molecular configurations might be used to carry and rectify electronic current. This notion was put forward well before its time, for today, some thirty years later, with the remarkable progress in nano tool development and material process capabilities, the concept of electronic conduction in molecular systems is now being experimentally tested in laboratories around the world. Correspondingly, over the years, there has been a substantial effort in the theoretical modeling of molecular configurations which has shed enormous light on the atomic details of the electron transport processes at the molecular level. The idea of considering electronic functionality at the molecular scale is not a surprise; it was very much embodied in Feynman's early vision captured in "There's Plenty of Room at the Bottom," and has always been part of the speculative horizon of Moore's law. Visionaries often speculate about the possibilities and opportunities to emerge from the molecular scale; but the challenges and barriers to success and realizability are substantial. The intention of this presentation is to discuss some of the basic possibilities and limitations of molecular scale electronics. Further, the presentation incorporates some of our recent quantum modelings on connected molecular systems; here we model metal contacts to molecular clusters in an *exact* framework using a molecular self-consistent field approach so as to calculate realistic, electric field dependent transport properties for the molecular system, and to study the role of the contact-molecule interface in influencing the transport properties of the entire molecular system.

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