Abstract: The recent advent of molecular electronic systems has opened up a new frontier, whose aim is the ultimate miniaturization of electronic systems. In this talk, the ideas and principles behind simulating the current-voltage (I-V) characteristics of such devices, at least at a density functional theory-based level will be reviewed. The focus will be on general principles important for transport. Specific topics to be discussed will be: (i) quantum transport through Si-cluster based systems; (ii) the role of evanescent modes in enhancing transport; and (iii) the capacitance characteristics of select carbon nanotube systems.