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Hierarchy of computational electronics approaches for multiscale charge transport simulation

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Semiconductor device simulation has been developed over several decades resulting in a hierarchy of computational electronics tools and approaches that are uniquely powerful for treating self-consistently the transport of charged particles. These methodologies, originally conceived for electronic transport in solid state systems, can be extended to other fields, particularly ionic transport in aqueous solutions, as found in biological systems. This talk will outline the hierarchy and the most important features of these transport model and discuss the new challenges encountered in treating general molecular systems as devices. Emphasis will be placed on discussing the approaches which are more suitable for future practical applications for engineering and design of molecular systems and devices, including multi-scale problems.