Exploring conductance switching properties of molecular scale devices - a computational approach.

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A computational approach is used and developed to study electron transport through molecular and nano scale devices. New models and methods to describe transient electron conductance through molecular systems under the influence of time dependent perturbations are used to study quantum interference effects affecting the time-dependent conductance. We also analyze several high-profile experimental studies achieving molecular scale conductance. The experiments demonstrate large conductance changes of single peptides upon ligation of proper metal ion or fabricated molecular sockets based on surface confined terpyridine ligands. Our calculations suggest structure-functions relations which have not been considered before.

References


