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**Exploring conductance switching properties of molecular scale devices - a computational approach.**[1] BARRY D. DUNIETZ, ALEXANDER PROCIUK, MOUSUMI DAS, TRILISA PERRINE, University of Michigan, DUNIETZ TEAM — A computational approach is used and developed to study electron transport through molecular scale devices. The study identifies and provides insight into mechanisms underlying transport switching properties. These systems include: 1. Spin-dependent electronic transport through a Porphyrin ring Ligating an Fe(II) atom, 2. Contact geometry and orientation effects of conjugated molecular transistors and 3. Chemical sensors with focus on metal recognition properties recently exhibited only for certain short peptide chains. The research also involves developing new models and methods to describe electron conductance through single molecular systems.

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