Exploring Conductance Switching Properties of Molecular Scale Devices - A Computational Approach.

A computational approach is used and developed to study electron transport through molecular scale devices. The study identifies and provides insight into mechanisms underlying electronic-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 field-effect 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 transient electron conductance through single molecular systems.

Host: Prof. Piotr Piecuch

October 2, 2007
Room 136 Chemistry
4:10 p.m.