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Theoretical study of hysteresis in electron transport through spin-crossover molecules KRISTEN BROWN, KYUNGWHA PARK, Dept. of Physics, Virginia Tech, Blacksburg, VA 24061 — Recent advances in nanoscale molecular systems stimulate experimental studies of electron transport across molecular junctions formed by single molecules or nanoparticles bridged between electrodes, or molecular monolayers adsorbed onto surfaces, using three-terminal set-ups or scanning tunneling microscope. Among them, spin-crossover molecular systems draw attention due to their unusual coupling between spin degrees of freedom and external stimuli. Spin magnetic moments of these molecular systems increase with increasing temperature or pressure, or shining light, and their magnetization shows hysteresis behavior with temperature, pressure, or light. Recent transport measurements across nanoparticles made of such spin-crossover molecules reveal hysteresis behavior in current-voltage characteristics, driven by voltage at a given temperature. In this talk, we present our work on understanding of hysteresis in electron transport through a nanoparticle consisting of Fe-based spin-crossover molecules, using a model-Hamiltonian approach and insight obtained from density functional theory.

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