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### **DFT-based Modeling of Field-Dependent Control and Response of Nanomagnetic Molecules<sup>1</sup>**

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Regardless of whether one is interested in characterizing, utilizing or controlling molecular-scale systems [1], one requisite to their understanding, design, and improvement is the ability to realistically model their response to electromagnetic fields. Since such responses are often collective their description requires an understanding of the interplay between bonding, spin, spin-orbit, vibrations, and electromagnetic fields. Inclusion of spin and magnetism influences the behaviors significantly. I provide an overview of a density-functional-based method (NRLMOL) for determining resonant tunneling of magnetization and Berry's phase oscillations in molecular magnets (primarily Mn<sub>12</sub>-Acetate and derivatives) [2] and spin-electric effects in frustrated spin systems [Na<sub>12</sub>Cu<sub>3</sub>(AsW<sub>9</sub>O<sub>33</sub>)<sub>2</sub>·3H<sub>2</sub>O] [3]. The complexities related to spin- and magnetically dependent transport are compared to those of a nonmagnetic case [4]. Direct comparisons to experiments will be made. Challenges and recent progress associated with incorporating these effects into a realistic description of the frequency and amplitude dependent field driven response of many-electron/spin nanosystems will be discussed.

[1] MRP and SN Khanna, PRB **60** 9566 (1999).

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