Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Vibrational properties of single-molecule magnet Fe4[1] MICHAEL WARNOCK, KYUNGWHA PARK, YOH YAMAMOTO, Virginia Tech — A single-molecule magnet (SMM) Fe_4 consists of four Fe ions interacting through O anions via antiferromagnetic superexchange coupling, with the total ground-state spin of $S = 5$. The SMM Fe_4 has a magnetic anisotropy energy of 16 K, and its ground-state spin multiplet is well separated from the first excited spin multiplet. A recent experimental effort demonstrated that SMMs Fe_4 can be deposited on various substrates with magnetic cores intact and that individual Fe_4 molecules can be bridged between electrodes. SMMs Fe_4 deposited on substrates or in contact with electrodes revealed interesting magnetic and transport properties. Electronic and spin degrees of freedom of SMM Fe_4 may be coupled to vibrational degrees of freedom. Such coupling can affect various properties of SMM Fe_4. Here we present our calculation of vibrational spectra (Raman and infrared) of SMM Fe_4 using density-functional theory (DFT) within simple harmonic oscillator approximation. We identify normal modes and compare our calculated result with available experimental data.

[1]This work was supported by NSF-DMR-0804665, 1206354, SDSC DMR060009N.

Michael Warnock
Virginia Tech

Date submitted: 08 Nov 2012 Electronic form version 1.4