

Abstract Submitted  
for the MAR12 Meeting of  
The American Physical Society

**Unification of ultrafast, laser-driven and slow, phonon-driven spin-flip scenarios in the three-magnetic-center cluster  $\text{Ni}_3\text{Na}_2$**  HONG-PING XIANG, GEORGIOS LEFKIDIS, WOLFGANG HÜBNER, Dept. of Physics and Research Center OPTIMAS, University of Kaiserslautern — Recently the use of the three-magnetic-center  $\text{Ni}_3\text{Na}_2$  on a fictitious, inert surface as a prototypical system for ultrafast, laser-driven spin manipulation and logic functionalization was reported [1]. Here we extend this investigation of spin dynamics on the same system by including vibronic motion and recalculating all electronic states for each structural distortion. The first immediate finding is that the system exhibits an unexpectedly rich set of magnetic phases (geometry sets with different orientations of the highly localized spin-density). Exploiting those phases allows us (a) to establish the combination of spin dynamics and phonons as an unprecedentedly accurate sensor of the bond length between metallic centers, and (b) to present for the first time a unified picture of ultrafast (fs), laser-driven and slow (ps), phonon-driven spin dynamics in molecular magnets.

[1] W. Hübner, S. Kersten, G. Lefkidis, Phys. Rev. B **79**, 184431 (2009).

Hongping Xiang  
Dept. of Physics and Research Center OPTIMAS,  
University of Kaiserslautern

Date submitted: 26 Nov 2011

Electronic form version 1.4