Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Two-stage orbital order and dynamical spin frustration in $KCuF_3$[1] JAMES C.T. LEE, Frederick Seitz Materials Research Laboratory (FSMRL), UIUC, SHI YUAN, FSMRL, UIUC, SIDDHARTHA LAL[2], FSMRL and Institute for Condensed Matter Theory (ICMT), UIUC, YOUNG-IL JOE, YU GAN, SERBAN SMADICI, FSMRL, UIUC, PAUL M. GOLDBART, FSMRL and ICMT, UIUC, S. LANCE COOPER, PETER ABBAMONTE, FSMRL, UIUC, KEN FINKELSTEIN, Cornell High Energy Synchrotron Source, Cornell University, YEJUN FENG, Advanced Photon Source, Argonne National Laboratory, ANDRIVO RUSYDI, National University of Singapore — Results from our x-ray and Raman scattering studies on $KCuF_3$, a model orbital order system, strongly link a low-temperature orbital order transition to a previously unidentified structural phase transition at 50 K. Raman scattering shows softening of phonon modes linked to F—ions that ceases upon a splitting of a degenerate E_g mode at 50 K. This, along with the emergence of diffuse scattering around an orbital order Bragg peak at low temperature, suggests an onset of $GdFeO_3$-like octahedral tilting, which serves to stabilize the Neel spin order at 39 K. To explain these effects, we have added to the Kugel-Khomskii model a term for direct orbital exchange driven by electron-electron interactions and ligand distortions. This term creates a near degeneracy, which dynamically frustrates the spin order at high temperature, that is lifted by orbital—lattice interactions at low temperature.

[1]Funding provided by grants from US DOE and NSF.
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Date submitted: 20 Dec 2011 Electronic form version 1.4