Abstract Submitted
for the MAR05 Meeting of
The American Physical Society

Spin frustration controlled by orbital fluctuations HIROAKI ONISHI, TAKASHI HOTTA, Advanced Science Research Center, Japan Atomic Energy Research Institute, Tokai, Ibaraki, 319-1195, Japan — In order to clarify a key role of orbital degree of freedom in geometrically frustrated electron systems, we investigate an $e_{\rm g}$-orbital Hubbard model on a zigzag chain at quarter filling by using numerical techniques. When two orbitals are degenerate, orbital degree of freedom is active, but a $3x^2 - r^2$ orbital is selectively occupied to suppress the spin frustration. Namely, the occupied orbital shape extends just along the direction of a double chain, and the zigzag chain is reduced to a double-chain spin system due to the spatial anisotropy of orbitals. On the other hand, taking account of the level splitting Δ between $3z^2 - r^2$ and $x^2 - y^2$ orbitals, electrons are forced to accommodate in the lower level. When the $3z^2 - r^2$ orbital is fully occupied for large positive Δ, the orbital anisotropy disappears in the xy plane and the spin frustration revives. With increasing Δ from zero to large values, the orbital state gradually changes and the orbital fluctuation is found to be significant in the intermediate region. We will discuss the change in orbital structure and spin incommensurability.

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Date submitted: 01 Dec 2004 Electronic form version 1.4