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Trimer Formation and Metal-Insulator Transition in Triangular-Lattice Systems LiVX_2 (X=O,Se,S) JUNKI YOSHITAKE, YUKITOSHI MOTOME, Dept. of Appl. Phys., Univ. of Tokyo — Geometrically-frustrated systems sometimes lift their degeneracy by spontaneous formation of multisite clusters via coupling to other degrees of freedom. A fascinating example is found in a triangular-lattice system $LiVO_2$, which exhibits a three-site trimer formation. The origin was argued to be an orbital ordering under strong electronic correlation [1], however, recent experiments on a series of LiVX_2 (X=O,Se,S) suggest that the system is intermediately correlated and rather close to a metal-insulator transition [2]. In this contribution,we revisit this problem within a multiorbital Hubbard model in a wide range of Coulomb interaction by strong-coupling perturbation and Hartree-Fock approximation. We find a new trimer state under substantial trigonal crystal-field splitting; it is located in the vicinity of a metal-insulator transition and not adiabatically connected to the trimer state previously proposed. We discuss the origin of this new trimerization and the relation to experimental results.

[1] H. F. Pen *et al.*, Phys. Rev. Lett. **78**, 1323 (1997).
[2] N. Katayama *et al.*, Phys. Rev. Lett. **103**, 146405 (2009).

Junki Yoshitake
Dept. of Appl. Phys., Univ. of Tokyo

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