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On metal-insulator transition in cubic fullerides NAOYA IWA-HARA, LIVIU CHIBOTARU, Theory of Nanomaterials Group, Katholieke Universiteit Leuven — The interplay between degenerate orbital and electron correlation is a key to characterize the electronic phases in, for example, transition metal compounds [1,2] and alkali-doped fullerides [3]. Besides, the degenerate orbital couples to spin and lattice degrees of freedom, giving rise to exotic phenomena. Here, we develop the self-consistent Gutzwiller approach for the simultaneous treatment of the Jahn-Teller effect and electron correlation, and apply the methodology to reveal the nature of the ground electronic state of fullerides [4]. For small Coulomb repulsion on site U, the fulleride is quasi degenerate correlated metal. With increase of U, we found the quantum phase transition from the metallic phase to JT split phase. In the latter, the Mott transition (MT) mainly develops in the half-filled subband, whereas the empty and the completely filled subbands are almost uninvolved. Therefore, we can qualify the metal-insulator transition in fullerides as an orbital selective MT [2] induced by JT effect. [1] Y. Tokura and N. Nagaosa, Science **288**, 462 (2000). [2] A. Koga, et al., Phys. Rev. Lett. **92**, 216402 (2004). [3] O. Gunnarsson, Rev. Mod. Phys. 69, 575 (1997). [4] N. Iwahara and L. F. Chibotaru, Phys. Rev. B 91, 035109 (2015).

> Naoya Iwahara Theory of Nanomaterials Group, Katholieke Universiteit Leuven

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