Abstract Submitted for the MAR12 Meeting of The American Physical Society

Ab initio Evidence of Strong Correlation Associated with Mott Proximity in Iron-Based Superconductor TAKAHIRO MISAWA, KAZUMA NAKAMURA, MASATOSHI IMADA, Dept. of Applied Physics, Univ. of Tokyo — Recently discovered iron-based superconductors have attracted much interest because of their high superconducting critical temperatures (T_c) . Although it is believed that electron correlations play key roles in the unconventional high- T_c superconductivity, their roles are not fully understood yet. To clarify electron correlation effects from a microscopic point of view, we study the *ab initio* low-energy effective models for iron-based superconductors by using multi-variable variational Monte Carlo (mVMC) method. From the *ab initio* calculations, we show that the iron-based superconductors found around d^6 configuration (namely, five Fe 3d orbitals filled by 6 electrons on average) are under the umbrella of an unexpectedly large-scale dome of correlated-electron matter centered at the Mott insulator at d^5 (namely, half filling). This proximity of the large-dome of strong electron correlations yields a variety with bad insulating (or incoherent metallic) states, quantum criticality of antiferromagnetism, orbital fluctuations and differentiations arising from interplay between the Hund's rule coupling and Mott physics.

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Date submitted: 11 Nov 2011

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