Abstract Submitted for the MAR17 Meeting of The American Physical Society

Topological Superconductivity on the Surface of Fe-Based Superconductors GANG XU, BIAO LIAN, PEIZHE TANG, XIAO-LIANG QI, SHOU-CHENG ZHANG, Stanford University — As one of the simplest systems for realizing Majorana fermions, the topological superconductor plays an important role in both condensed matter physics and quantum computations. Based on *ab initio* calculations and the analysis of an effective 8-band model with superconducting pairing, we demonstrate that the three-dimensional extended s-wave Fe-based superconductors such as  $Fe_{1+y}Se_{0.5}Te_{0.5}$  have a metallic topologically nontrivial band structure, and exhibit a normal-topological-normal superconductivity phase transition on the (001) surface by tuning the bulk carrier doping level. In the topological superconductivity (TSC) phase, a Majorana zero mode is trapped at the end of a magnetic vortex line. We further show that the surface TSC phase only exists up to a certain bulk pairing gap, and there is a normal topological phase transition driven by the temperature, which has not been discussed before. These results pave an effective way to realize the TSC and Majorana fermions in a large class of superconductors.

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Date submitted: 15 Dec 2016

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