Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Microscopic origin of dissipative two-level systems in Al_2O_3[1]
LUKE GORDON, Univ of California - Santa Barbara, HAZEM A. FARSAKH, Prince Sultan University, Saudi Arabia, ANDERSON JANOTTI, CHRIS G. VAN DE WALLE, University of California, Santa Barbara — Resonant absorption of two-level systems (TLS) poses a serious limitation to the performance of superconducting qubit devices for quantum computing. Experiments indicate that the TLS is associated with defects in the dielectric layers of the device. However, the nature of these defects has yet to be established. Using hybrid functional calculations, we investigate possible defects in Al_2O_3 that can act as sources of resonant absorption. Hydrogen is a ubiquitous impurity, and easily incorporates in the interstitial sites (H_i) in Al_2O_3. In the positive charge state, H_i is bonded to one oxygen atom, but also interacts with a secondary oxygen atom. At particular O-O distances, close to those found in amorphous Al_2O_3 or near the Al_2O_3/Al interface, the H atom is effectively in a double well. We calculate the three-dimensional potential energy surface (PES) for the H atom in a so-called "coincidence configuration," which allows for tunneling between two equivalent positions. Using the calculated PES, we solve the Schrödinger equation for the tunneling proton and determine the tunneling frequency. We find that H_i gives rise to resonant absorption in the range of 10-100 GHz, in agreement with experimental observations.

[1]This work was supported by IARPA

Luke Gordon
Univ of California - Santa Barbara

Date submitted: 14 Nov 2013 Electronic form version 1.4