Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Paramagnetic Spins on -Al_2O_3 with Varied Surface Termination[1]

KEITH RAY, Lawrence Livermore National Laboratory, DONGHWA LEE, Chonnam National University, NICOLE ADELSTEIN, San Francisco State University, JONATHAN DUBOIS, VINCENZO LORDI, Lawrence Livermore National Laboratory — Superconducting qubits (SQs) are promising building blocks for a quantum computer, however, coherence in SQs is reduced by unintended coupling to magnetic noise sources. The microscopic origins of the magnetic noise have not been satisfactorily characterized. Building on previous computational studies [PRL 112, 017001 (2014)] of magnetic spins induced by molecules adsorbed on bare Al terminated Al2O3, we present a density functional theory investigation of magnetic noise associated with other Al2O3 surfaces likely to be encountered in experiment. We calculate the exchange interaction between native defects and adsorbed molecules, as well as the magnetic states energy splitting and anisotropy, on fully hydroxylated Al2O3, with and without a water over-layer. We also present simulated x-ray adsorption and x-ray magnetic circular dichroism spectra of these systems with the aim of aiding experimental surface characterization.

[1]This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under contract DE-AC52-07NA27344.

Keith Ray
Lawrence Livermore National Laboratory

Date submitted: 06 Nov 2015 Electronic form version 1.4