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Paramagnetic Spin Dynamics on Different Terminations of Al2O3[1] KEITH RAY, JONATHAN DUBOIS, VINCENZO LORDI, Lawrence Livermore National Laboratory — Superconducting qubits are susceptible to magnetic flux noise which reduces their coherence through dephasing. The microscopic origins of the observed magnetic flux noise have not been fully characterized. Questions remain as to where the most relevant spins reside that couple to the qubit, the nature of the spin-spin coupling in realistic materials, and the behavior of the resulting spin system dynamics. Paramagnetic O2 has been previously identified experimentally as a likely flux noise source [Phys. Rev. Applied 6, 041001 (2016)] and computational studies [PRL 112, 017001 (2014)] of magnetic spins induced by molecules adsorbed on bare Al-terminated Al2O3 demonstrated the possibility of nearly degenerate adsorbate magnetic states. Here, we present a density functional theory investigation of magnetic noise associated with other Al2O3 surfaces likely to be encountered in experiment. Motivated by noise models involving spin clusters on the surface, we calculate the exchange interaction between adsorbed molecules, OH groups and paramagnetic O2, as well as the magnetic state energy splitting and anisotropy, on fully hydroxylated and Al terminated Al2O3. We use the calculated magnetic quantities to parametrize Monte Carlo models that characterize the spin dynamics, taking into account the disorder of absorbed O2 molecules that define a spin lattice.

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