Abstract Submitted
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Identification of the microscopic origin of unpaired surface spins on superconducting devices using XMCD simulations[1] ZHE WANG, State Key Laboratory of Surface Physics, Key Laboratory of Computational Physical Sciences, and Department of Physics, Fudan University, Shanghai, HUI WANG, CLARE YU, RUQIAN WU, Department of Physics and Astronomy, University of California, Irvine — Unpaired surface spins reside on superconducting quantum interference devices (SQUIDs) are significant sources of the 1/f flux noise, which limits the coherence time of superconducting devices. Recently, the x-ray magnetic circular dichroism (XMCD) technique has been successfully used to identify the species of these unpaired spins, where adsorbed molecular O2 was demonstrated to be the dominant contributor. Here, we present systematic density functional theory (DFT) investigations on the XMCD spectra of adsorbed O2 and other likely candidates include dangling bonds, surface vacancies. Pronounced peaks can be found in the x-ray absorption and XMCD spectra due to the transition from the 1s core to $2\pi^*$ orbitals; and the peak intensity decreases when the bond direction of O2 molecule deviates away from the incident x-rays. In contrast, the XMCD signals from the lattice are either zero or in much higher energy position, indicating that the XMCD technique can be used in detecting the origin of unpaired spins on qubits.

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