Band offset modulation in Si-EuO heterostructures *via* controlled interface formation

W. Li, A. Posadas, and A. A. Demkov
Department of Physics, The University of Texas at Austin, Austin, TX, 78712, USA

In a Si-based spintronic device, Si serves as the spin channel material. Owing to its small spin-orbit coupling, Si has a long spin relaxation lifetime and long spin coherence length, making it an excellent choice. Because the rock salt lattice of EuO is compatible with the ***fcc*** lattice of Si (see Fig. 1), and EuO is thermodynamically stable on Si, Si/EuO heterostructures have a real potential for use in Si-based spin-FETs. Combining first principles calculations and experiment, we investigate the atomic and electronic structure of the Si/EuO interface. We consider the thermodynamic stability of interface structures with different levels of oxidation to identify the most probable configuration. By comparing the calculated band alignment and core level shifts with measured values, we validate the theoretically constructed interface model. EuO has unusual electronic properties in that its charge neutrality level appears to be inside the conduction band [1,2]. In Fig. 2 we show a contour plot of the partial density of states (PDOS) as a function of energy and position along the *z* direction normal to the plane of the interface. In the contour plot one can clearly see the band edges of Si and EuO and read off the VBO, which is +0.19 eV. We find that the band offset can be tuned by altering the relative energy positions of the Si and EuO conduction bands via interface oxidation, which can be used to tune this materials system for specific applications in spintronics [3].

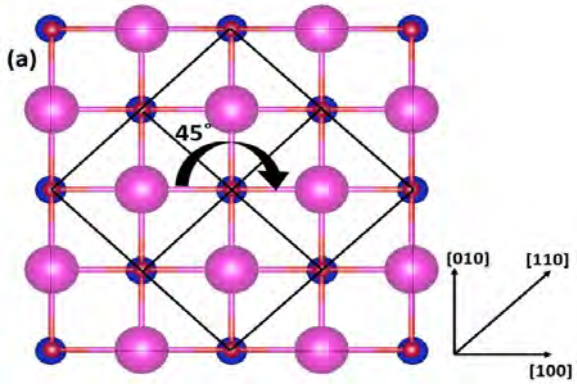

Figure 1. Top view of rock salt EuO and face centered silicon lattices. Purple ball represents Eu, red O and blue Si. It can be seen that rocksalt and face centered lattices match well. It can also be rotated by 45°.

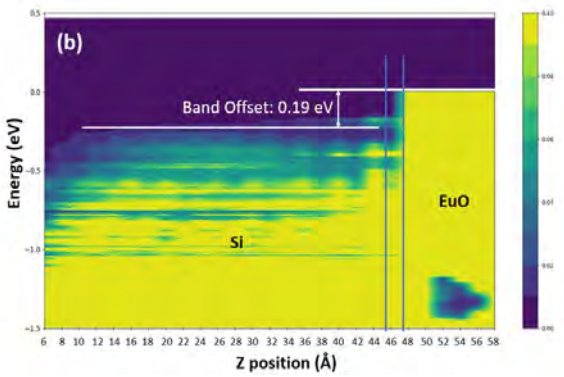

Figure 2. Contour plot of PDOS for spin-up channel in the valence band and band gap regions. The dark blue region is the band gap and the yellow region is the valence band top.

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[2] L. Gao, W. Guo, A. B. Posadas and A. A. Demkov, Phys. Rev. Materials **3**, 094403 (2019).
[3] W. Li, A. B. Posadas, and A. A. Demkov, *in press*, Phys. Rev. B (2019).

[+] Author for correspondence: demkov@physics.utexas.edu