

# A new type of magnetic tunnel junction based on spin filtering through a reduced symmetry oxide

## (Supporting Information)

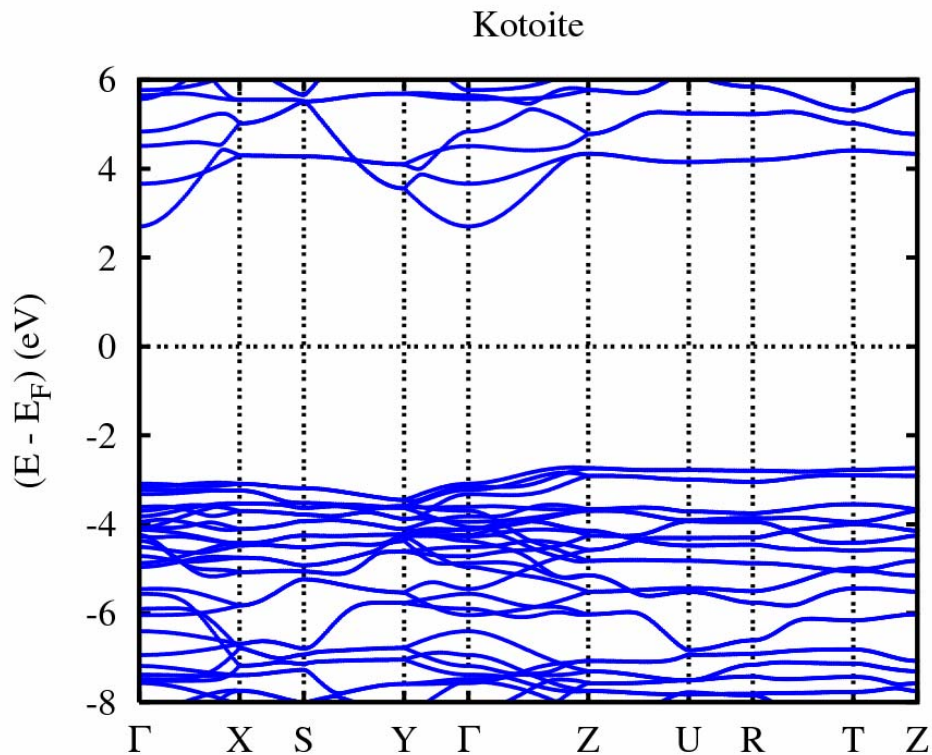
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Mg <sub>3</sub> B <sub>2</sub> O <sub>6</sub> Atomic Positions		
Atom	Calculated Fractional Coordinates	Experimental Fractional Coordinates Ref[11]
Mg1	(0.0000, 0.0000, 0.0000)	(0.0000, 0.0000, 0.0000)
Mg2	(0.0000, 0.3136, 0.5000)	(0.0000, 0.3128, 0.5000)
B	(0.2579, 0.0000, 0.5461)	(0.2546, 0.0000, 0.5453)
O1	(0.3239, 0.0000, 0.2513)	(0.3222, 0.0000, 0.2502)
O2	(0.2051, 0.1389, 0.7007)	(0.2045, 0.1387, 0.7029)

**Table S1.** This table compares the calculated fractional coordinates with measured values<sup>11</sup> for unique atoms in the orthorhombic unit cell of Kotoite (Mg<sub>3</sub>B<sub>2</sub>O<sub>6</sub>).



**Figure S1.** The band diagram of Kotoite (Mg<sub>3</sub>B<sub>2</sub>O<sub>6</sub>) calculated using the Augmented Spherical Wave approach.

For the augmented spherical wave calculations of Kotoite, lattice vectors and atomic positions were taken from the relaxed plane wave calculation done with the Quantum Espresso code. Empty spheres were also included to account for the open nature of the Kotoite. The number and location of the empty spheres was determined using an automatic procedure in the Augmented Spherical Wave code. For the self-consistent calculations, a Monkhorst k-grid of 11x7x13 was used.