Supplementary Information

Electric Field Tunable Half-Metallic Characteristic at
Fe₃O₄/BaTiO₃ Interfaces

Xueyao Hou¹, Xiaocha Wang², Guifeng Chen³, Wenbo Mi¹,¹

¹Tianjin Key Laboratory of Low Dimensional Materials Physics and Preparation
Technology & Key Laboratory of Advanced Ceramics and Machining Technology of
Ministry of Education, Faculty of Science, Tianjin University, 300354, Tianjin, China

²School of Electronics Information Engineering, Tianjin University of Technology,
300384, Tianjin, China

³School of Material Science and Engineering, Hebei University of Technology,
300130, Tianjin, China

*Author to whom all correspondence should be addressed.
E-mail: miwenbo@tju.edu.cn
Table. S1. Bader charges of bulk Fe₃O₄, TiO-Fe₅B₃O (solid lines) and OTi-Fe₅B₃O (dash lines).

<table>
<thead>
<tr>
<th>Bader charge (e)</th>
<th>unstrained FO</th>
<th>5% FO</th>
<th>TiO-Fe₅B₃O</th>
<th>OTi-Fe₅B₃O</th>
</tr>
</thead>
<tbody>
<tr>
<td>O</td>
<td>-0.81</td>
<td>-0.80</td>
<td>-1.09</td>
<td>-1.11</td>
</tr>
<tr>
<td>Feₐ</td>
<td>+1.49</td>
<td>+1.62</td>
<td>1.65</td>
<td>1.61</td>
</tr>
<tr>
<td>Feₐ</td>
<td>+1.65</td>
<td>+1.59</td>
<td>1.62</td>
<td>1.50</td>
</tr>
</tbody>
</table>
Fig. S1. The potentials of TiO-Fe$_B$O and OTi-Fe$_B$O along $z$ direction.
Fig. S2. The spin-resolved band structure of bulk BaTiO$_3$, the high-symmetry points are $\Gamma$ (0, 0, 0), $X$ (0, 0.5, 0), $M$ (0.5, 0.5, 0), $A$ (0.5, 0.5, 0.5).
Fig. S3. DOS of the III-O and III-Ti of the two models with different electric fields, the color of line were plot on the right.
**Fig. S4.** The spin-up band structures of TiO-FeB\(_2\)O (top panel) and OTi-FeB\(_2\)O (bottom panel) with different electric fields.
Fig. S5. (a), (d) The displacements of TiO and Fe\textsubscript{B}O of TiO-Fe\textsubscript{B}O and TiO-Fe\textsubscript{B}O with different electric fields; (b) or (c) is $M_{FeA}$ ($M_{FeB}$) as functional of layers in TiO-Fe\textsubscript{B}O with different electric fields; (e), (f) are responding $M_{FeA}$ ($M_{FeB}$) in OTi-Fe\textsubscript{B}O.