Supporting materials for "Impact of Sr segregation on the electronic structure and oxygen reduction activity of SrTi_{1-x}Fe_xO₃ surfaces"

Yan Chen,^a WooChul Jung,^{b,c} Zhuhua Cai,^a Jae Jin Kim,^b Harry L. Tuller^b and Bilge Yildiz*^a

^a Laboratory for Electrochemical Interfaces, Department of Nuclear Science and Engineering, Massachusetts Institute of Technology, Cambridge, MA 02139, USA. ; Fax: 617-258-8863; Tel: 617-324-4009; E-mail: byildiz@mit.edu

^b Department of Materials Science and Engineering, Massachusetts Institute of Technology, Cambridge, MA 02139, USA.

^c Present address: Department of Materials Science, California Institute of Technology, Cambridge, MA 02159, C

* byildiz@mit.edu

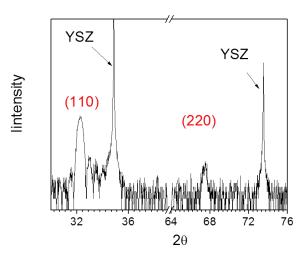


Fig. S1: Representative high resolution x-ray diffraction pattern of the $SrTi_{1-x}Fe_xO_3$ films in this work, showing highly textured structure in the (110) out-of-plane direction. The specific data shown here is from the STF35 film.

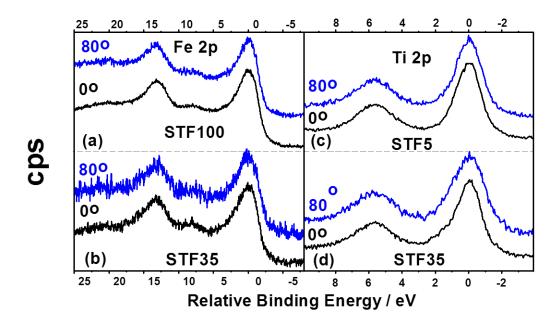


Fig. S2: (a-b) Comparison of the Fe 2p spectra in the bulk (0°) and on the surface (80°) of SrTi_{0.65}Fe_{0.35}O₃ (STF35) and SrFeO₃ (STF100). (c-d) Comparison of the Ti 2p spectra in the bulk (0°) and on the surface (80°) of SrTi_{0.95}Fe_{0.05}O₃ (STF5) and SrTi_{0.65}Fe_{0.35}O₃ (STF35).

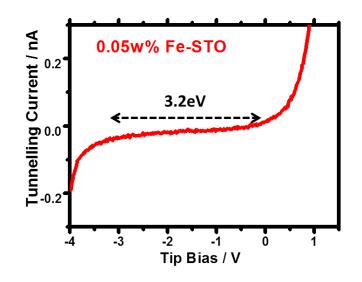


Fig. S3 : The tunneling current versus tip bias data on 0.05 w% Fe-doped SrTiO₃ single crystal substrate (from MTI Corporation, Richmond, CA) at 345°C, $P_{o2}\sim10^{-3}$ mbar. The Fermi level is closer to the top of valence band (positive tip bias), which is consistent with the acceptor doped nature of the sample. The small slope existing in the tunneling spectra within the range of from 0 to -3.2 eV closely represents the band gap of SrTiO₃. The non-zero slope of the tunneling current within the band gap energy range is due to the defect states created within the gap at high temperature and/or with Fe doping.

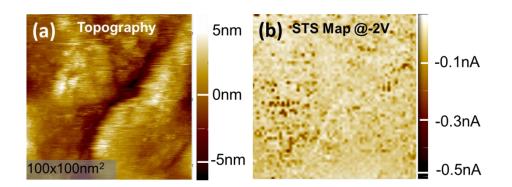


Fig. S4 : (a) Topography image taken by scanning tunneling microscopy and (b) tunneling current map measured by scanning tunneling spectroscopy on $SrTi_{0.95}Fe_{0.05}O_3$ (STF5) at 345°C, $P_{o2}\sim10^{-3}$ mbar. No clear correlation between structural features, e. g. grain boundaries, and the tunneling current magnitude is found.

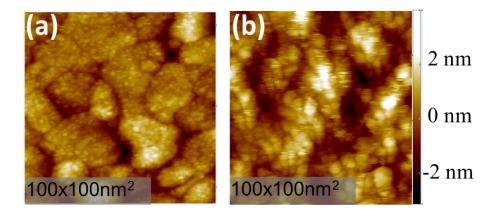


Fig. S5: Surface structure of the SrTi_{0.65}Fe_{0.35}O₃ (STF35) measured by scanning tunneling microscopy at 345°C, P_{O2} ~ 1×10⁻³ (a) before chemical etching, and (b) after chemical etching (using 0.14 mol/l HCl for 10 s).