Support Information

A formation mechanism of oxygen vacancies in a MnO₂ monolayer: A DFT+U study

Chenghua Sun,* Yong Wang, Jin Zou, Sean C. Smith

Received (in XXX, XXX) Xth XXXXXXXXX 200X, Accepted Xth XXXXXXXXX 200X
First published on the web Xth XXXXXXXXX 200X
DOI: 10.1039/b000000x

Centre for Computational Molecular Science, Australian Institute of Bioengineering and Nanotechnology, The University of Queensland, QLD 4072, Brisbane, Australia. Fax: 617 3346 3992; Tel: 617 3346 3949; E-mail: s.smith@uq.edu.au (S.C. Smith); c.sun1@uq.edu.au (C.H. Sun)
Materials Engineering and Centre for Microscopy Microanalysis, The University of Queensland, QLD 4072, Australia

S1: Side view of MnO₂ monolayer (4×4×1 supercell)

Fig. S1 Side view of perfect MnO₂ nanosheets modelled by 4×4×1 supercell. Mn and O are indicated by purple and red spheres.

S2: Models of 8×8×1 supercell (top view)

Fig. S2 Perfect MnO₂ nanosheets modelled by 8×8×1 supercell. Mn and O are indicated by purple and red spheres.
S3: Calculated reaction energies from $8 \times 8 \times 1$ supercell

**Fig. S3** Reaction energies ($E_r$) for the release of neutral oxygen molecules and oxygen ions ($O^{2-}$) calculated from the $8 \times 8 \times 1$ supercell with $U = 4.0$ eV.