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Support Information

A formation mechanism of oxygen vacancies in a MnO_2 monolayer: A DFT+U study

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

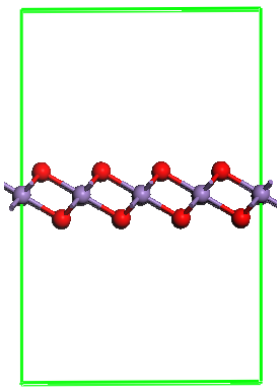

Fig. S1 Side view of perfect MnO_2 nanosheets modelled by 4×4×1 supercell. Mn and O are indicated by purple and red spheres.

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

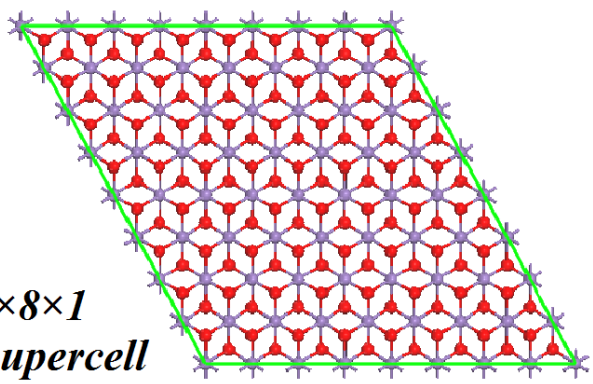

Fig. S2 Perfect MnO_2 nanosheets modelled by 8×8×1 supercell. Mn and O are indicated by purple and red spheres..

S3: Calculated reaction energies from 8×8×1 supercell

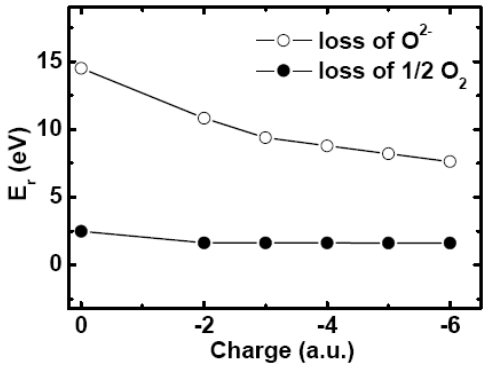

Fig. S3 Reaction energies (Er) for the release of neutral oxygen molecules and oxygen ions (O^{2-}) calculated from the 8×8×1 supercell with U = 4.0 eV.