Electronic supplementary material for:

Structure and spectroscopy of the supercapacitor material hydrous ruthenium oxide, RuO2.*x*H2O, by neutron scattering

Stewart F Parkera\* Stephen J. Robertsonb and Silvia Imbertia

aISIS Facility, STFC Rutherford Appleton Laboratory, Chilton, Didcot, OX11 0QX, UK

b*Advanced Material Group, STFC Rutherford Appleton Laboratory, Chilton, Didcot, Oxfordshire, OX11 0QX, UK*

E-mail: [stewart.parker@stfc.ac.uk](mailto:stewart.parker@stfc.ac.uk)

Table S1 describes the various models of the surface species on RuO2(110), a comparison of the INS spectrum of RuO2.0.99.H2O with that calculated from the models are shown in Figures S1 – S9. The model used is shown as an inset in each figure.

**Table S1.** Description of the surface structures investigated.



|  |  |  |  |
| --- | --- | --- | --- |
| Model and Figure number | Sites occupied |  | Number of imaginary modes |
|  | Ru-cus | O-bridge |  |
| 1 | None | H vertical | 2 |
| 2 | None | H tilted | 0 |
| 3 | O–H H-bonded to O-bridge | None | 0 |
| 4 | O–H oriented along [001] | Doubly protonated to H2O | 2 |
| 5 | H2O | H vertical | 6 |
| 6 | H2O | H tilted | 0 |
| 7 | Alternating H2O and O–H oriented along [001]a | None | 2 |
| 8 | O–H oriented along [001] | None | 0 |
| 9 | O–H oriented along [001] | H2O H-bonded to O-bridge and Ru–O–H | 0 |

a [001] is along the direction of O-bridge.



**Figure S1.** Blue trace: INS spectrum of RuO2.0.99H2O, Red trace: INS spectrum calculated for calculated for Model 1 of the surface species present on Ru(110) (see Table S1 for details), Olive trace: as red trace but broadened to mimic surface disorder.

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**Figure S2.** Blue trace: INS spectrum of RuO2.0.99H2O, Red trace: INS spectrum calculated for calculated for Model 2 of the surface species present on Ru(110) (see Table S1 for details), Olive trace: as red trace but broadened to mimic surface disorder.

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**Figure S3.** Blue trace: INS spectrum of RuO2.0.99H2O, Red trace: INS spectrum calculated for calculated for Model 3 of the surface species present on Ru(110) (see Table S1 for details), Olive trace: as red trace but broadened to mimic surface disorder.



**Figure S4.** Blue trace: INS spectrum of RuO2.0.99H2O, Red trace: INS spectrum calculated for calculated for Model 4 of the surface species present on Ru(110) (see Table S1 for details), Olive trace: as red trace but broadened to mimic surface disorder.



**Figure S5.** Blue trace: INS spectrum of RuO2.0.99H2O, Red trace: INS spectrum calculated for calculated for Model 5 of the surface species present on Ru(110) (see Table S1 for details), Olive trace: as red trace but broadened to mimic surface disorder.



**Figure S6.** Blue trace: INS spectrum of RuO2.0.99H2O, Red trace: INS spectrum calculated for calculated for Model 6 of the surface species present on Ru(110) (see Table S1 for details), Olive trace: as red trace but broadened to mimic surface disorder.



**Figure S7.** Blue trace: INS spectrum of RuO2.0.99H2O, Red trace: INS spectrum calculated for calculated for Model 7 of the surface species present on Ru(110) (see Table S1 for details), Olive trace: as red trace but broadened to mimic surface disorder.



**Figure S8.** Blue trace: INS spectrum of RuO2.0.99H2O, Red trace: INS spectrum calculated for calculated for Model 8 of the surface species present on Ru(110) (see Table S1 for details), Olive trace: as red trace but broadened to mimic surface disorder.



**Figure S9.** Blue trace: INS spectrum of RuO2.0.99H2O, Red trace: INS spectrum calculated for calculated for Model 9 of the surface species present on Ru(110) (see Table S1 for details), Olive trace: as red trace but broadened to mimic surface disorder.