**Supplementary Materials**

A Non-Noble Cr-Ni based Catalyst for the Oxygen Reduction Reaction in Alkaline Polymer Electrolyte Fuel Cells

P. Faubert1#, I. Kondov2, J. Erben3, D.Qazzazie4, O. Yurchenko5, C. Müller1

1 University of Freiburg, Department of Microsystems Engineering IMTEK, Laboratory for

Process Technology, D-79110 Freiburg, Germany

2 Steinbuch Centre for Computing, Karlsruhe Institute of Technology, Hermann-von-Helmholtz-

Platz 1, 76344 Eggenstein-Leopoldshafen, Germany

3 University of Freiburg, Department of Microsystems Engineering IMTEK, Laboratory for

MEMS Applications, D-79110 Freiburg, Germany

4 University of Freiburg, Department of Microsystems Engineering IMTEK, Laboratory for

Sensors, D-79110 Freiburg, Germany

5 University of Freiburg, Freiburg Materials Research Center FMF, D-79104 Freiburg, Germany

# Corresponding Author / E-mail: [patrick.faubert@imtek.uni-](mailto:patrick.faubert@imtek.uni-)freiburg.de, Tel: +49 (0)761 / 203-7359

Table S1: Effective reversible potentials *U*eff, critical potentials *U*max, (in V vs. RHE) and the rate determining step (RDS) according to reactions (4) and (5) for the ORR at a vacancy site of various surface structures on Ni (111) with and without Cr modifications. Asterisks (\*) denote the positions of the ORR active sites. The structure notations refer to Fig. 1.

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Structure | Doping | Decoration | O-Coverage | CrOx | *U*max | *U*0 ˗ *U*max | *U*eff | *U*eff ˗ *U*max | RDS |
| 0AB\*DD'D"F'F" | 0 | 0 | 7/16 | 0 | 0.17 | 1.06 | 0.18 | 0.01 | 4 |
| 0AB\*B'B"DF'F" | 0 | 0 | 7/16 | 0 | 0.21 | 1.02 | 0.86 | 0.65 | 4 |
| 0AB'B"C\*DF'F" | 0 | 0 | 7/16 | 0 | 0.13 | 1.10 | 0.16 | 0.03 | 5 |
| 0AB\*B'B"CDF'F" | 0 | 0 | 1/2 | 0 | 0.19 | 1.04 | 0.85 | 0.66 | 4 |
| 0ABB'B"C\*DF'F" | 0 | 0 | 1/2 | 0 | 0.13 | 1.10 | 0.15 | 0.03 | 5 |
| 0ABB'B"C\*DD'D" | 0 | 0 | 1/2 | 0 | 0.16 | 1.07 | 0.64 | 0.48 | 4 |
| 1B | 1/16 | 0 | 1/4 | 3/16 | 0.09 | 1.14 | 0.20 | 0.11 | 4 |
| 1C | 1/16 | 0 | 1/4 | 3/16 | 0.07 | 1.16 | 0.15 | 0.08 | 4 |
| 1A\*BC | 1/16 | 0 | 6/16 | 3/16 | 0.23 | 1.00 | 0.43 | 0.20 | 4 |
| 1AB\*C | 1/16 | 0 | 6/16 | 3/16 | 0.11 | 1.12 | 0.15 | 0.04 | 4 |
| 1ABC\* | 1/16 | 0 | 6/16 | 3/16 | 0.17 | 1.06 | 0.17 | 0.00 | 4 |
| 1AB\*D'D" | 1/16 | 0 | 7/16 | 3/16 | 0.11 | 1.12 | 0.15 | 0.03 | 4 |
| 1ABD'\*D" | 1/16 | 0 | 7/16 | 3/16 | 0.20 | 1.03 | 0.49 | 0.30 | 4 |
| 1ABCD'\* | 1/16 | 0 | 7/16 | 3/16 | 0.25 | 0.98 | 0.68 | 0.43 | 4 |
| 3C\* | 3/16 | 0 | 7/16 | 6/16 | 0.08 | 1.15 | 0.16 | 0.08 | 4 |
| 3E'\* | 3/16 | 0 | 7/16 | 6/16 | 0.19 | 1.04 | 0.52 | 0.33 | 4 |
| 3B\* | 3/16 | 0 | 7/16 | 6/16 | 0.25 | 0.98 | 0.82 | 0.57 | 4 |
| 3B\*C | 3/16 | 0 | 1/2 | 6/16 | 0.28 | 0.95 | 0.78 | 0.50 | 4 |
| 3BC\* | 3/16 | 0 | 1/2 | 6/16 | 0.12 | 1.11 | 0.12 | 0.00 | 4 |
| 3C\*E' | 3/16 | 0 | 1/2 | 6/16 | 0.17 | 1.06 | 0.35 | 0.18 | 4 |
| 3CE'\* | 3/16 | 0 | 1/2 | 6/16 | 0.24 | 0.99 | 0.71 | 0.47 | 4 |
| 1B\* | 0 | 1/16 | 1/4 | 3/16 | 0.14 | 1.09 | 0.14 | 0.00 | 5 |
| 1C\* | 0 | 1/16 | 1/4 | 3/16 | 0.12 | 1.11 | 0.13 | 0.02 | 5 |
| 1A\* | 0 | 1/16 | 1/4 | 3/16 | 0.15 | 1.07 | 0.18 | 0.03 | 5 |
| 1AB\*C | 0 | 1/16 | 6/16 | 3/16 | 0.11 | 1.12 | 0.14 | 0.02 | 5 |
| 1A\*BC | 0 | 1/16 | 6/16 | 3/16 | 0.13 | 1.10 | 0.19 | 0.06 | 5 |
| 1A\*B'B"C | 0 | 1/16 | 7/16 | 3/16 | 0.38 | 0.85 | 0.58 | 0.21 | 4 |
| 1AB'B"C\* | 0 | 1/16 | 7/16 | 3/16 | 0.12 | 1.11 | 0.15 | 0.04 | 5 |
| 3B\* | 0 | 3/16 | 1/2 | 7/16 | 0.16 | 1.07 | 0.19 | 0.03 | 5 |
| 3C\* | 0 | 3/16 | 1/2 | 7/16 | 0.24 | 0.99 | 0.26 | 0.03 | 5 |
| 3BC\* | 0 | 3/16 | 9/16 | 7/16 | 0.27 | 0.96 | 0.28 | 0.01 | 5 |
| 3B\*C | 0 | 3/16 | 9/16 | 7/16 | 0.14 | 1.09 | 0.20 | 0.06 | 5 |
| 2B\* | 1/16 | 1/16 | 7/16 | 6/16 | 0.11 | 1.12 | 0.14 | 0.03 | 5 |
| 2C\* | 1/16 | 1/16 | 7/16 | 6/16 | 0.29 | 0.94 | 0.41 | 0.12 | 4 |
| 2B\*C | 1/16 | 1/16 | 1/2 | 6/16 | 0.18 | 1.05 | 0.18 | 0.00 | 4 |
| 2BC\* | 1/16 | 1/16 | 1/2 | 6/16 | 0.30 | 0.93 | 0.45 | 0.15 | 4 |

****

FIG. S1: SEM/BSE image of the carbon fiber supported Cr-Ni electrode. Carbon fibers with Cr-Ni particles within the carbon fibers developed by electro spun proves.



FIG. S2: Working principle of the electro spinning process.



FIG. S3: Surface structures used in the simulations. Only the topmost three slab layers are shown as viewed along the axis perpendicular to the surface. Atoms with no labels are always included in the structures, atoms with labels are included only if indicated in the structure descriptions in Table 1. The orange line denotes the unit cell.