

## Description of Additional Supplementary Files

### Supplementary Data 1.

**Description:** Pt (111), Pt (111) model with \*O intermediate at top site during ORR process, Pt (111) model with \*O intermediate at hollow site during ORR process, Pt (111) model with \*O intermediate at bridge site during ORR process, defect free PZFCNC-HEI, PD-PZFCNC-HEI, PD-PZFCNC-HEI-1 site 1 (Pt-PtCoNiPtPtZn) model for ORR, PD-PZFCNC-HEI-1 site 2 (Zn-CrPtPtPtPtPt) model for ORR, PD-PZFCNC-HEI-2 model for ORR, and PD-PZFCNC-HEI-3 model for ORR reported in this manuscript.