

## Supporting Information

### Theoretical insight into the catalytic activities of the oxygen reduction reaction on the transition metal-N<sub>4</sub> doped graphene

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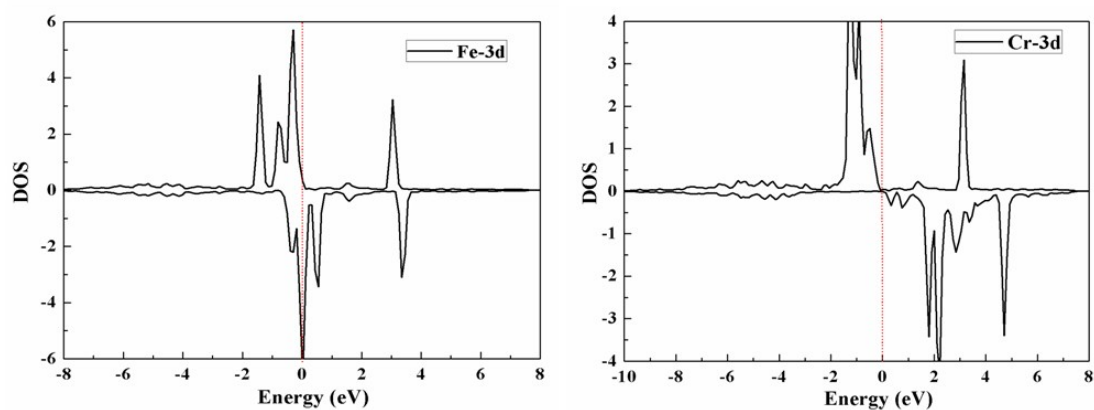
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**Table S1.** The free energy changes of  $\Delta G_x$  ( $x=1-4$ ) in ORR on M-N<sub>4</sub>-C

|    | $\Delta G_1$ | $\Delta G_2$ | $\Delta G_3$ | $\Delta G_4$ |
|----|--------------|--------------|--------------|--------------|
| Cr | -3.33        | -1.56        | -0.07        | 0.04         |
| Mn | -1.21        | -2.37        | -0.79        | -0.55        |
| Fe | -1.88        | -2.16        | -0.74        | -0.14        |
| Co | -0.83        | -1.39        | -1.59        | -1.11        |
| Ni | 0.003        | -0.95        | -1.91        | -2.06        |
| Ru | -1.91        | -2.36        | -0.62        | -0.03        |
| Rh | -0.79        | -1.42        | -1.57        | -1.14        |
| Pd | 0.30         | -0.63        | -2.16        | -2.43        |
| Os | -2.40        | -2.61        | 0.007        | 0.08         |
| Ir | -0.78        | -1.82        | -1.16        | -1.16        |
| Pt | 0.12         | -0.66        | -1.90        | -2.48        |

**Table S2.** Bader charge on metal, nitrogen and the ten nearest carbon atoms (C-10) surrounding the M-N<sub>4</sub> moiety. NC is the sum of the MN<sub>4</sub> and C-10.

|    | Metal | N <sub>4</sub> | C-10 | NC    |
|----|-------|----------------|------|-------|
| Cr | 1.25  | -4.80          | 3.37 | -0.18 |
| Mn | 1.28  | -5.09          | 3.42 | -0.39 |
| Fe | 1.00  | -4.99          | 3.42 | -0.57 |
| Co | 0.84  | -4.94          | 3.44 | -0.66 |
| Ni | 0.82  | -4.93          | 3.46 | -0.65 |
| Mo | 1.27  | -5.17          | 3.55 | -0.35 |
| Tc | 1.24  | -5.03          | 3.35 | -0.44 |
| Ru | 0.90  | -4.89          | 2.97 | -1.02 |
| Rh | 0.61  | -4.84          | 3.10 | -1.13 |
| Pd | 0.70  | -4.80          | 3.06 | -1.04 |
| Os | 0.93  | -4.71          | 2.73 | -1.05 |
| Ir | 0.73  | -4.67          | 2.88 | -1.06 |
| Pt | 0.72  | -4.75          | 2.99 | -1.04 |



**Fig. S1.** Density of states for Fe-N<sub>4</sub>-C and Cr-N<sub>4</sub>-C. The vertical red line is the Fermi Level.