

## Supporting information

### Theoretical screening of the metal-nonmetal pair anchored on N-doped Graphene for Oxygen Reduction Reaction

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Number of tables: 1

Number of figures: 3

Table S1. The calculated over potentials and the Gibbs free energy changes for each step of ORR on SM@N<sub>8</sub> catalysts.

| slab | $\Delta G_{\text{OOH}}$ | $\Delta G_{\text{O}}$ | $\Delta G_{\text{OH}}$ | Over potential |
|------|-------------------------|-----------------------|------------------------|----------------|
| STi  | 0.19                    | -2.38                 | -2.53                  | 3.76           |
| SV   | 0.68                    | -1.93                 | -1.69                  | 2.92           |
| SCr  | 2.69                    | 0.04                  | -0.36                  | 1.59           |
| SMn  | 2.93                    | 0.92                  | 0.10                   | 1.13           |
| SFe  | 3.18                    | 1.47                  | 0.49                   | 0.74           |
| SCo  | 3.85                    | 2.69                  | 1.15                   | 0.40           |
| SNi  | 4.35                    | 3.47                  | 1.64                   | 0.90           |
| SCu  | 3.89                    | 3.05                  | 1.06                   | 0.44           |
| SZn  | 3.30                    | 2.53                  | -0.22                  | 1.45           |
| SZr  | -1.05                   | -4.07                 | -4.40                  | 5.63           |
| SNb  | -0.95                   | -3.54                 | -3.31                  | 4.54           |
| SMo  | 0.01                    | -2.69                 | -1.92                  | 3.15           |
| SRu  | 2.43                    | 0.64                  | -0.25                  | 1.48           |
| SRh  | 3.88                    | 2.90                  | 1.21                   | 0.43           |
| SPd  | 4.42                    | 4.28                  | 2.08                   | 0.97           |
| SAg  | 2.49                    | 2.04                  | -0.17                  | 1.40           |
| SCd  | 2.06                    | 1.21                  | -1.92                  | 3.15           |
| SHf  | -1.02                   | -3.77                 | -4.45                  | 5.68           |
| STa  | -1.09                   | -3.85                 | -3.75                  | 4.98           |
| SW   | -0.49                   | -3.23                 | -3.15                  | 4.38           |
| SRe  | 0.41                    | -2.24                 | -1.66                  | 2.89           |
| SOs  | 2.05                    | 0.01                  | -0.56                  | 1.79           |
| SIr  | 3.74                    | 2.44                  | 0.99                   | 0.29           |
| SPt  | 4.48                    | 4.13                  | 1.93                   | 1.03           |
| SAu  | 4.20                    | 4.05                  | 1.42                   | 0.84           |
| SHg  | 0.99                    | -0.52                 | -2.59                  | 3.82           |
| PNi  | 4.03                    | 3.18                  | 1.31                   | 0.58           |
| PCu  | 3.66                    | 2.86                  | 0.79                   | 0.44           |
| PIr  | 3.39                    | 1.68                  | 0.34                   | 0.89           |
| OIr  | 1.09                    | -0.43                 | -1.90                  | 3.13           |

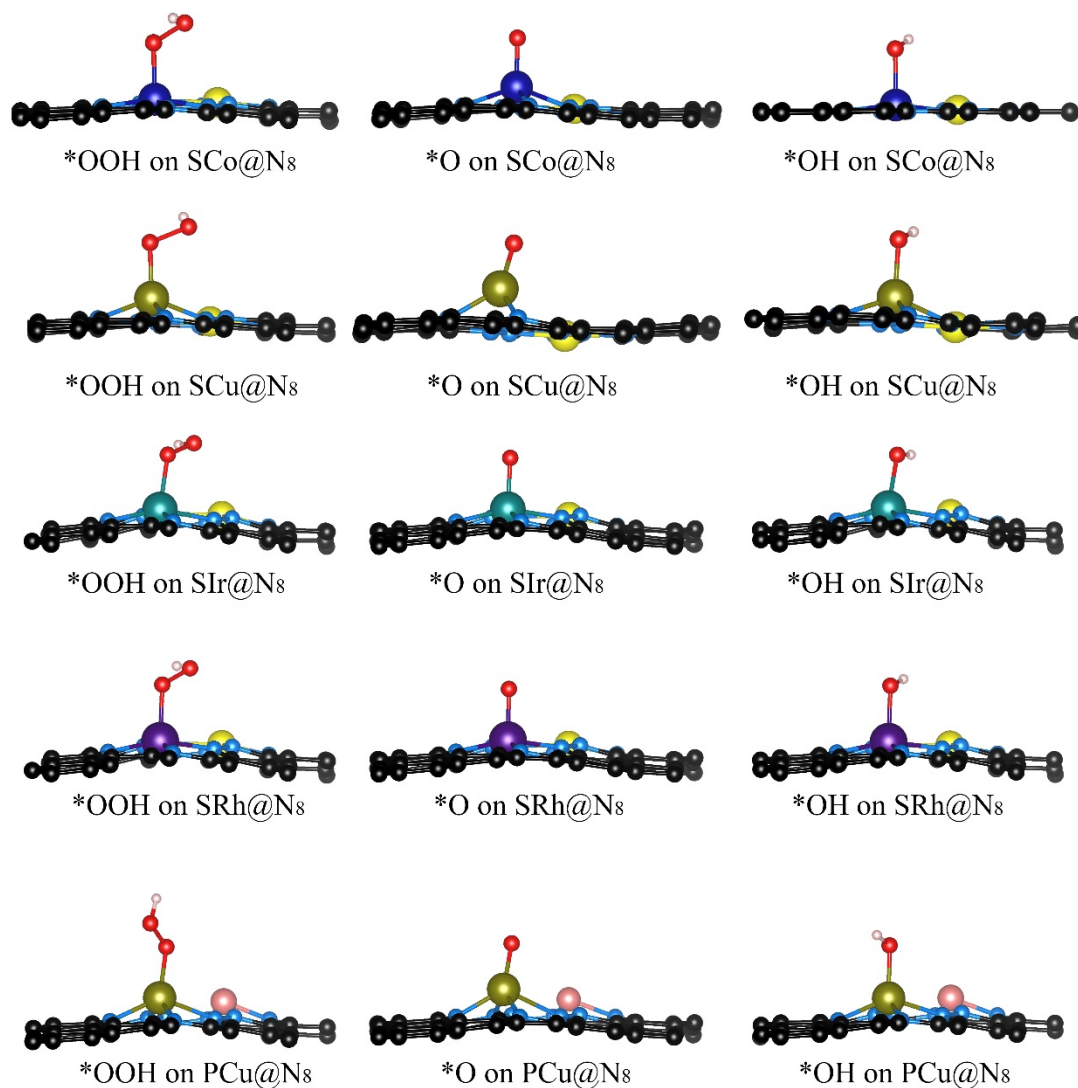


Figure S1. The relaxed geometry of intermediates, such as OOH, O and OH, adsorbed on SCo, SCu, SRh, SIr and PCu catalysts.

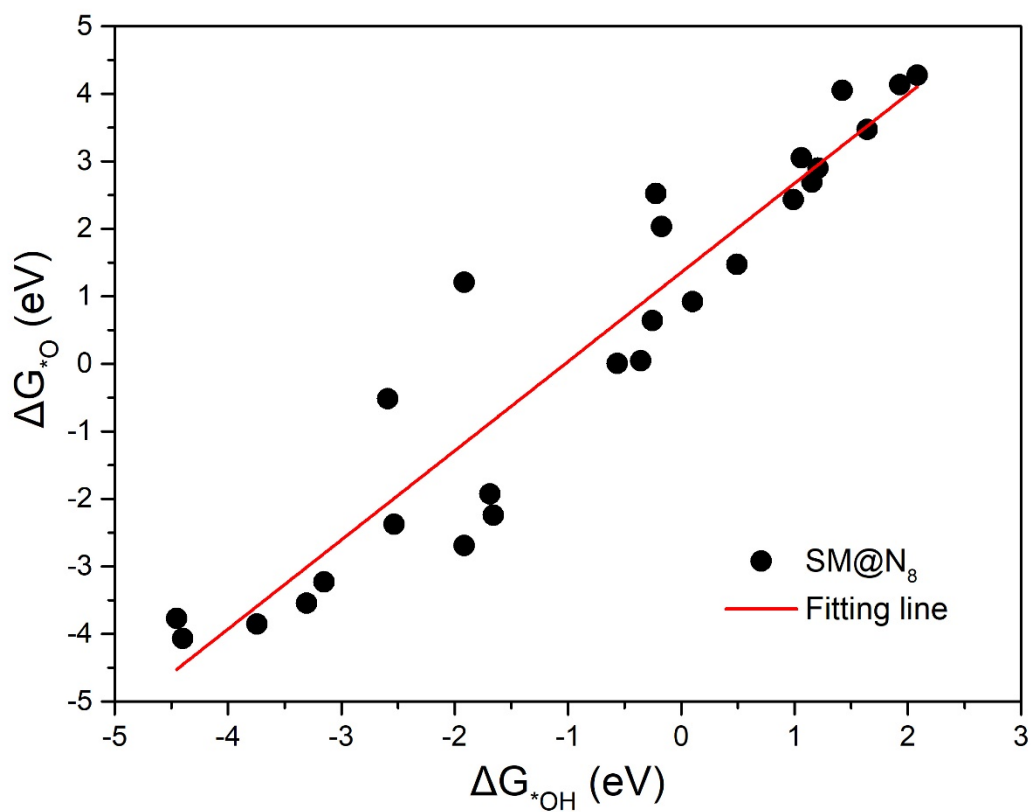


Figure S2. Scaling relationships of adsorption free energy for  $\text{*O}$  vs  $\text{*OH}$  species on  $\text{SM@N}_8$ . The linear fitting was expressed as  $\Delta G_{\text{*OH}} = 1.32\Delta G_{\text{*O}} + 1.35$  and shown in red solid line with R-square of 0.89.

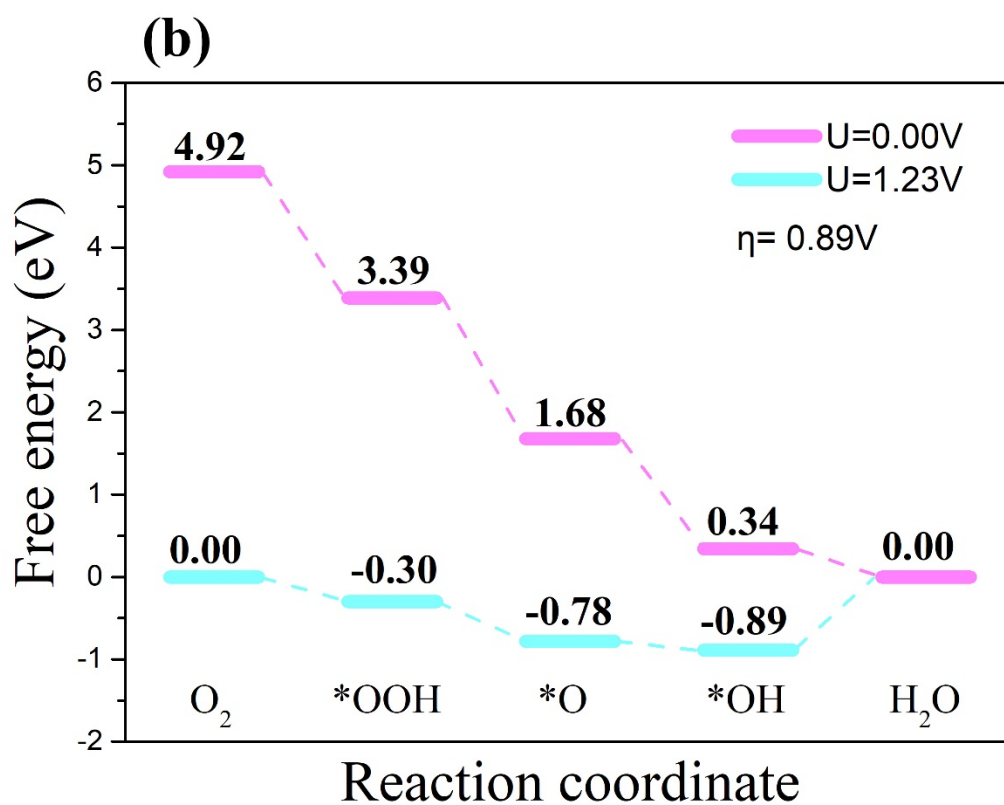
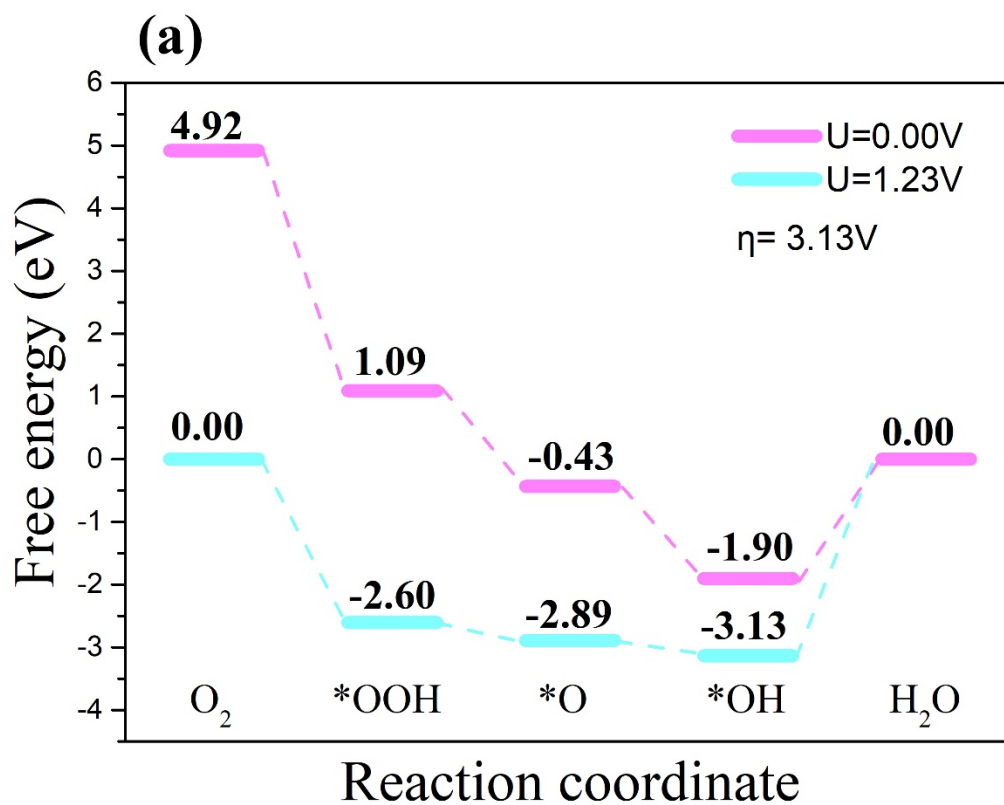


Figure S3. Energy profiles of the reaction on (a) OIr and (b) PIr catalysts

