Supporting Information for

"Catalytic Activity Trends of Pyrite Transition
Metal Dichalcogenides for Oxygen Reduction
and Evolution"

Wooseok Lee\textsuperscript{a}, Jongseung Kim\textsuperscript{a}, Heejin Kim\textsuperscript{b,*} and Seoin Back\textsuperscript{a,*}

\textsuperscript{a} Department of Chemical and Biomolecular Engineering, Institute of Emergent Materials, Sogang University, Seoul 04107, Republic of Korea

\textsuperscript{b} Division of Analytical Science, Korea Basic Science Institute (KBSI), Yuseong-gu, Daejon 34133, Republic of Korea
**Supplementary Note: \( U-J (U_{\text{eff}}) \) Values for TMDs**

To determine appropriate \( U-J \) values for calculating ORR/OER catalytic activity of pyrite TMDs systems, four strategies were considered as listed below.

1. **\( U-J (U_{\text{eff}}) \) values from previous literature**

   Most frequently, \( U-J \) values (or \( U_{\text{eff}} \)) were taken from the previous literature, where the previous literature calculated those values by fitting experimental values of by using a linear response approach, which will be discussed in the following. A summary of various \( U-J \) values used for pyrite TMDs and the corresponding references are in Table S4 and Table S5. As indicated in Table S4 and Table S5, there is no consensus in \( U-J \) values for pyrite TMDs even though same functional was used.

2. **\( U-J (U_{\text{eff}}) \) values from Materials Project**

   The largest database of inorganic materials, The Materials Project\(^1\), determined \( U-J \) values by fitting experimental formation enthalpies. We note that U-correction was only applied for oxide materials and all TMDs were treated by PBE in the Materials Project database. Since not all experimental formation enthalpies of TMDs are available, thus this strategy is not applicable for TMDs.

3. **\( U-J (U_{\text{eff}}) \) values from experimental results**

   When experimental photoelectron spectroscopy (PES) or bandgap values are available, \( U-J \) values that most closely reproduce experimental values were chosen\(^2\). For TMDs considered in this work, bandgap values of only five out of twelve TMDs have been reported and Co-based TMDs are known to be metallic, thus this approach is not applicable either.

4. **\( U-J (U_{\text{eff}}) \) values from linear response method**

   Linear response method proposed by Cococcioni and Gironcoli\(^3\) is conventionally used for its good reproducibility of experimental results. In this approach, the effective U parameters (\( U_{\text{eff}} \)) are calculated from the difference between the inverse bare (non-interacting) density response, \( \chi^{-1} \), and the inverse self-consistent (interacting) density response, \( \chi^{-0} \). We split metal atoms into two groups (atom 1, and atom 2-32) and included small perturbations (\( \pm 0.08, \pm 0.05, \pm 0.02 \) eV) to atom 1 with \( 2\times2\times2 \) supercell consisting of 96 atoms (containing 32 metal atoms and 64 chalcogen atoms) to avoid errors induced by interactions between perturbations and their periodic images. Using the determined \( U_{\text{eff}} \) values, we performed bulk optimizations and compared the lattice parameters with experimental results (Table S6). Notably, the percent difference
in the lattice parameters was found to be significant, especially for Fe and Co based TMDs.

As discussed above, several approaches were either unavailable due to the lack of experimental data or incapable of reproducing experimental values.

Surface catalytic processes are significantly affected by geometric and electronic properties\textsuperscript{4}. For the former, since the surface catalytic processes are accompanied by the adsorption, cleavage and association of reactant molecules, the geometric parameters of active sites can alter the binding geometry and energy, thus impacting the catalytic activity prediction. In this point of view, the validity of the lattice parameter is essential for estimating the activity of materials.

Thus, we fitted $U_{\text{eff}}$ with respect to the experimental lattice parameters. Although this approach is not perfect either, it reproduced some of experimental catalytic results for TMDs. For example, our computational method predicted CoSe$_2$ and CoTe$_2$ to be active for OER in agreement with the experimental literature\textsuperscript{5, 6}. 
Figure S1. The percentage value of the average difference between experimentally measured and DFT calculated lattice parameters of Mn-based TMDs (MnS$_2$, MnSe$_2$ and MnTe$_2$) with varying $U_{eff}$ values.

Figure S2. (a) Side and (b) top view of (001) TMD surface structures. Color codes: pink (metal) and yellow (chalcogen). Marked atoms were fixed during the geometry optimization.
**Figure S3.** Seven different surface coverages considered to construct the surface Pourbaix diagrams, where M indicates metal sites (Mn, Fe, Co, Ni) and Ch indicates chalcogen sites (S, Se, Te).

**Figure S4.** The surface Pourbaix diagrams for (001) surface of all TMDs. (a) MnS₂, (b) MnSe₂, (c) MnTe₂, (d) FeS₂ (e) FeSe₂ (f) FeTe₂ (g) CoS₂ (h) CoSe₂ (i) CoTe₂ (j) NiS₂ (k) NiSe₂ and (l) NiTe₂. In all cases, O*-covered (M-O*/Ch-O*, purple) surfaces are found to be
most stable under both ORR (blue dashed line) and OER (red dashed line) operating conditions. Black dashed line indicates the equilibrium potential of ORR/OER.

Figure S5. Pearson correlation coefficient matrix of all features considered in this work. The color bar represents correlation coefficients between two features. Explanations of features can be found in Table S3.
Figure S6. Projected density of states (PDOS) of bulk (a) MnS$_2$, (b) MnSe$_2$, (c) MnTe$_2$, (d) FeS$_2$, (e) FeSe$_2$, (f) FeTe$_2$, (g) CoS$_2$, (h) CoSe$_2$, (i) CoTe$_2$, (j) NiS$_2$, (k) NiSe$_2$ and (l) NiTe$_2$. Green and purple colors correspond to PDOS of transition metals and chalcogens, respectively. The black dashed line indicates the Fermi energy.
Figure S7. Binding free energies of $\Delta G_{{O^*}}$ and $\Delta G_{{OOH^*}}$ plotted with respect to $\Delta G_{{OH^*}}$ when chalcogen sites are considered as adsorption sites. No scaling relation was observed. The lower $\Delta G$ indicates stronger binding.

Figure S8. Comparisons of scaling relations for TMD (001) surfaces (black lines) with respect to the conventional scaling relations for transition metals and metal oxides\(^7\) (red dashed lines). (a) $\Delta G_{{O^*}}$ vs $\Delta G_{{OH^*}}$ and (b) $\Delta G_{{OOH^*}}$ vs $\Delta G_{{OH^*}}$. 
Figure S9. Two-dimensional volcano plots for predicting (a) ORR and (b) OER overpotentials with respect to different equilibrium potential ($U_{eq}$), 1.11 V of DFT level of theory (left) or 1.23 V of experimental value (right).
Table S1. A summary of DFT calculated and experimentally measured lattice parameters of bulk TMDs. The percentage difference was calculated referenced to the experimental values. PBE+U ($U_{eff} = 3$ eV) was used only for the relaxation of Mn-based TMDs.

<table>
<thead>
<tr>
<th>TMDs</th>
<th>DFT calculated lattice parameter (Å)</th>
<th>Experimentally measured lattice parameter (Å)</th>
<th>Difference (%)</th>
<th>Ref</th>
</tr>
</thead>
<tbody>
<tr>
<td>MnS$_2$</td>
<td>6.18</td>
<td>6.10</td>
<td>1.3</td>
<td>8</td>
</tr>
<tr>
<td>MnSe$_2$</td>
<td>6.54</td>
<td>6.42</td>
<td>1.9</td>
<td>9</td>
</tr>
<tr>
<td>MnTe$_2$</td>
<td>7.06</td>
<td>6.94</td>
<td>1.6</td>
<td>10</td>
</tr>
<tr>
<td>FeS$_2$</td>
<td>5.41</td>
<td>5.40</td>
<td>0.1</td>
<td>8</td>
</tr>
<tr>
<td>FeSe$_2$</td>
<td>5.80</td>
<td>5.79</td>
<td>0.3</td>
<td>11</td>
</tr>
<tr>
<td>FeTe$_2$</td>
<td>6.27</td>
<td>6.29</td>
<td>-0.4</td>
<td>11</td>
</tr>
<tr>
<td>CoS$_2$</td>
<td>5.51</td>
<td>5.53</td>
<td>-0.4</td>
<td>12</td>
</tr>
<tr>
<td>CoSe$_2$</td>
<td>5.85</td>
<td>5.85</td>
<td>0.0</td>
<td>12</td>
</tr>
<tr>
<td>CoTe$_2$</td>
<td>6.32</td>
<td>6.32</td>
<td>-0.1</td>
<td>11</td>
</tr>
<tr>
<td>NiS$_2$</td>
<td>5.60</td>
<td>5.68</td>
<td>-1.4</td>
<td>8</td>
</tr>
<tr>
<td>NiSe$_2$</td>
<td>5.94</td>
<td>5.96</td>
<td>-0.3</td>
<td>13</td>
</tr>
<tr>
<td>NiTe$_2$</td>
<td>6.42</td>
<td>6.37</td>
<td>0.8</td>
<td>11</td>
</tr>
</tbody>
</table>

Table S2. The ground state DFT energy of TMD bulk systems in antiferromagnetic (AFM) and ferromagnetic (FM) orderings and their differences per formula unit. Energy units are in eV/formula unit.

<table>
<thead>
<tr>
<th>TMDs</th>
<th>AFM</th>
<th>FM</th>
<th>Energy difference (eV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>MnS$_2$</td>
<td>-69.18</td>
<td>-68.90</td>
<td>0.07</td>
</tr>
<tr>
<td>MnSe$_2$</td>
<td>-63.43</td>
<td>-63.19</td>
<td>0.06</td>
</tr>
<tr>
<td>MnTe$_2$</td>
<td>-58.09</td>
<td>-57.85</td>
<td>0.06</td>
</tr>
<tr>
<td>FeS$_2$</td>
<td>-72.12</td>
<td>-72.12</td>
<td>0.00</td>
</tr>
<tr>
<td>FeSe$_2$</td>
<td>-64.97</td>
<td>-64.97</td>
<td>0.00</td>
</tr>
<tr>
<td>FeTe$_2$</td>
<td>-59.76</td>
<td>-59.76</td>
<td>0.00</td>
</tr>
<tr>
<td>CoS$_2$</td>
<td>-65.51</td>
<td>-65.51</td>
<td>0.00</td>
</tr>
<tr>
<td>CoSe$_2$</td>
<td>-59.56</td>
<td>-59.55</td>
<td>0.00</td>
</tr>
<tr>
<td>CoTe$_2$</td>
<td>-55.28</td>
<td>-55.28</td>
<td>0.00</td>
</tr>
<tr>
<td>NiS$_2$</td>
<td>-57.90</td>
<td>-57.85</td>
<td>0.01</td>
</tr>
<tr>
<td>NiSe$_2$</td>
<td>-52.74</td>
<td>-52.73</td>
<td>0.00</td>
</tr>
<tr>
<td>NiTe$_2$</td>
<td>-49.15</td>
<td>-49.14</td>
<td>0.00</td>
</tr>
</tbody>
</table>
**Table S3.** The ground state magnetic moment per metal atom for bulk structures.

<table>
<thead>
<tr>
<th>TMDs</th>
<th>Magnetic Moment (μB)</th>
<th>Magnetic ordering</th>
</tr>
</thead>
<tbody>
<tr>
<td>MnS$_2$</td>
<td>4.43</td>
<td>AFM</td>
</tr>
<tr>
<td>MnSe$_2$</td>
<td>4.42</td>
<td>AFM</td>
</tr>
<tr>
<td>MnTe$_2$</td>
<td>4.39</td>
<td>AFM</td>
</tr>
<tr>
<td>FeS$_2$</td>
<td>0</td>
<td>NM</td>
</tr>
<tr>
<td>FeSe$_2$</td>
<td>0</td>
<td>NM</td>
</tr>
<tr>
<td>FeTe$_2$</td>
<td>0</td>
<td>NM</td>
</tr>
<tr>
<td>CoS$_2$</td>
<td>0.89</td>
<td>FM</td>
</tr>
<tr>
<td>CoSe$_2$</td>
<td>0.78</td>
<td>FM</td>
</tr>
<tr>
<td>CoTe$_2$</td>
<td>0.41</td>
<td>FM</td>
</tr>
<tr>
<td>NiS$_2$</td>
<td>0.56</td>
<td>AFM</td>
</tr>
<tr>
<td>NiSe$_2$</td>
<td>0.03</td>
<td>AFM</td>
</tr>
<tr>
<td>NiTe$_2$</td>
<td>0</td>
<td>NM</td>
</tr>
</tbody>
</table>

**Table S4.** Summary of U−J values (eV) chosen previously.

<table>
<thead>
<tr>
<th>TMDs</th>
<th>Functional</th>
<th>U−J values (eV)</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>MnS$_2$</td>
<td>PBE + U</td>
<td>3.9, 2</td>
<td>14, 15</td>
</tr>
<tr>
<td>MnSe$_2$</td>
<td>PBE + U</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>MnTe$_2$</td>
<td>PBE + U</td>
<td>4.2</td>
<td>16</td>
</tr>
<tr>
<td>FeS$_2$</td>
<td>PBE + U</td>
<td>2, 1.2, 1.8</td>
<td>17-19</td>
</tr>
<tr>
<td>FeSe$_2$</td>
<td>PBE + U</td>
<td>3.3</td>
<td>20</td>
</tr>
<tr>
<td>FeTe$_2$</td>
<td>PBE + U</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>CoS$_2$</td>
<td>PBE + U</td>
<td>4, 2, 5</td>
<td>21-23</td>
</tr>
<tr>
<td>CoSe$_2$</td>
<td>PBE + U</td>
<td>1, 2, 3</td>
<td>24-26</td>
</tr>
<tr>
<td>CoTe$_2$</td>
<td>PBE + U</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>NiS$_2$</td>
<td>PBE + U</td>
<td>4.5, 6.39</td>
<td>27, 28</td>
</tr>
<tr>
<td>NiSe$_2$</td>
<td>PBE + U</td>
<td>4.39, 3.4</td>
<td>28, 29</td>
</tr>
<tr>
<td>NiTe$_2$</td>
<td>PBE + U</td>
<td>-</td>
<td>-</td>
</tr>
</tbody>
</table>

**Table S5.** Summary of the previous studies which used PBE functional.

<table>
<thead>
<tr>
<th>TMDs</th>
<th>Functional</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>MnS$_2$</td>
<td>PBE</td>
<td>30</td>
</tr>
<tr>
<td>MnSe$_2$</td>
<td>PBE</td>
<td>31</td>
</tr>
<tr>
<td>MnTe$_2$</td>
<td>PBE</td>
<td>32</td>
</tr>
<tr>
<td>FeS$_2$</td>
<td>PBE</td>
<td>30</td>
</tr>
<tr>
<td>FeSe$_2$</td>
<td>PBE</td>
<td>33</td>
</tr>
<tr>
<td>FeTe$_2$</td>
<td>PBE</td>
<td>-</td>
</tr>
<tr>
<td>CoS$_2$</td>
<td>PBE</td>
<td>30, 34-36</td>
</tr>
<tr>
<td>CoSe$_2$</td>
<td>PBE</td>
<td>31, 37, 38</td>
</tr>
<tr>
<td>CoTe$_2$</td>
<td>PBE</td>
<td>39</td>
</tr>
<tr>
<td>NiS$_2$</td>
<td>PBE</td>
<td>30</td>
</tr>
<tr>
<td>NiSe$_2$</td>
<td>PBE</td>
<td>31</td>
</tr>
<tr>
<td>NiTe$_2$</td>
<td>PBE</td>
<td>40</td>
</tr>
</tbody>
</table>
Table S6. Summary of $U_{\text{eff}}$ calculated using linear response approach and the corresponding lattice differences with respect to the experimental values.

<table>
<thead>
<tr>
<th>TMDs</th>
<th>Linear response $U_{\text{eff}}$ (eV)</th>
<th>Lattice difference (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>MnS$_2$</td>
<td>6.02</td>
<td>1.95</td>
</tr>
<tr>
<td>MnSe$_2$</td>
<td>5.92</td>
<td>2.48</td>
</tr>
<tr>
<td>MnTe$_2$</td>
<td>5.68</td>
<td>2.52</td>
</tr>
<tr>
<td>FeS$_2$</td>
<td>5.05</td>
<td>3.26</td>
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<tr>
<td>FeSe$_2$</td>
<td>5.00</td>
<td>6.46</td>
</tr>
<tr>
<td>FeTe$_2$</td>
<td>4.90</td>
<td>6.28</td>
</tr>
<tr>
<td>CoS$_2$</td>
<td>6.40</td>
<td>4.59</td>
</tr>
<tr>
<td>CoSe$_2$</td>
<td>6.46</td>
<td>4.39</td>
</tr>
<tr>
<td>CoTe$_2$</td>
<td>6.02</td>
<td>4.86</td>
</tr>
<tr>
<td>NiS$_2$</td>
<td>6.20</td>
<td>2.11</td>
</tr>
<tr>
<td>NiSe$_2$</td>
<td>6.34</td>
<td>3.23</td>
</tr>
<tr>
<td>NiTe$_2$</td>
<td>6.11</td>
<td>4.14</td>
</tr>
</tbody>
</table>

Table S7. Free energy correction values for gas-phase molecules (H$_2$ and H$_2$O) and adsorbates (O*, OH* and OOH*) calculated using the ideal gas and harmonic oscillator approximation, respectively, as implemented in Atomic Simulation Environment (ASE)$^{41}$. Partial pressures of H$_2$ and H$_2$O were set to 101,325 and 3,534 Pa, respectively. All values are in eV.

<table>
<thead>
<tr>
<th></th>
<th>ZPE</th>
<th>$-\text{TS}$</th>
<th>$\int C_p dT$</th>
</tr>
</thead>
<tbody>
<tr>
<td>H$_2$ (g)</td>
<td>0.26</td>
<td>-0.40</td>
<td>0.09</td>
</tr>
<tr>
<td>H$_2$O (g)</td>
<td>0.57</td>
<td>-0.66</td>
<td>0.11</td>
</tr>
<tr>
<td>O*</td>
<td>0.06</td>
<td>-0.07</td>
<td>0.04</td>
</tr>
<tr>
<td>OH*</td>
<td>0.34</td>
<td>-0.10</td>
<td>0.06</td>
</tr>
<tr>
<td>OOH*</td>
<td>0.41</td>
<td>-0.12</td>
<td>0.06</td>
</tr>
</tbody>
</table>

Table S8. Symbols and definitions of features used in linear regressions.

<table>
<thead>
<tr>
<th>Elementary atomic properties</th>
<th>Bulk properties</th>
</tr>
</thead>
<tbody>
<tr>
<td>$EN_M$ Electronegativity of metal atom</td>
<td>$IP_M$ Ionization potential of metal atom</td>
</tr>
<tr>
<td>$EN_C$ Electronegativity of chalcogen atom</td>
<td>$IP_C$ Ionization potential of chalcogen atom</td>
</tr>
<tr>
<td>$Ea_M$ Electron affinity of metal atom</td>
<td>$R_M$ Covalent radius of metal atom</td>
</tr>
<tr>
<td>$Ea_C$ Electron affinity of chalcogen atom</td>
<td>$R_C$ Covalent radius of chalcogen atom</td>
</tr>
<tr>
<td>#3$d$ Number of outer d-electrons in the metal atom</td>
<td>$q_M$ Bader charge of metal atom</td>
</tr>
<tr>
<td>#3$d_U$ Number of unpaired electrons in the metal atom</td>
<td>$M-Ch$ Metal-Chalcogen bond length</td>
</tr>
</tbody>
</table>
Table S9. Top 10 combinations of features for the linear model sorted by the average value of mean absolute error (MAE) for $\Delta G_{O^*}$ and $\Delta G_{OH^*}$ predictions.

<table>
<thead>
<tr>
<th>Combinations</th>
<th>Average MAE (eV)</th>
<th>Average R$^2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$[Ea_M, q_M]$</td>
<td>0.13</td>
<td>0.89</td>
</tr>
<tr>
<td>$[#3d, q_M]$</td>
<td>0.16</td>
<td>0.84</td>
</tr>
<tr>
<td>$[Ea_M, R_M]$</td>
<td>0.23</td>
<td>0.67</td>
</tr>
<tr>
<td>$[EN_M, #3d_U]$</td>
<td>0.23</td>
<td>0.67</td>
</tr>
<tr>
<td>$[#3d, #3d_U]$</td>
<td>0.23</td>
<td>0.66</td>
</tr>
<tr>
<td>$[#3d, Ea_M]$</td>
<td>0.23</td>
<td>0.66</td>
</tr>
<tr>
<td>$[EN_M, Ea_M]$</td>
<td>0.24</td>
<td>0.65</td>
</tr>
<tr>
<td>$[#3d, R_M]$</td>
<td>0.24</td>
<td>0.65</td>
</tr>
<tr>
<td>$[#3d, EN_M]$</td>
<td>0.24</td>
<td>0.65</td>
</tr>
</tbody>
</table>

Table S10. The binding free energies of $O^*$, $OH^*$, $OOH^*$, the calculated ORR and OER overpotentials and the corresponding potential limiting steps (PLS).

<table>
<thead>
<tr>
<th>TMDs</th>
<th>Binding Free Energies</th>
<th>ORR</th>
<th>OER</th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$\Delta G(O)$</td>
<td>$\Delta G(OH)$</td>
<td>$\Delta G(OOH)$</td>
<td>$\eta^{\text{ORR}}$</td>
<td>PLS</td>
</tr>
<tr>
<td>MnS$_2$</td>
<td>2.81</td>
<td>0.88</td>
<td>3.98</td>
<td>0.35</td>
<td>OH$^*$→H$_2$O</td>
</tr>
<tr>
<td>MnSe$_2$</td>
<td>2.74</td>
<td>0.74</td>
<td>3.80</td>
<td>0.49</td>
<td>OH$^*$→H$_2$O</td>
</tr>
<tr>
<td>MnTe$_2$</td>
<td>2.47</td>
<td>0.56</td>
<td>3.61</td>
<td>0.67</td>
<td>OH$^*$→H$_2$O</td>
</tr>
<tr>
<td>FeS$_2$</td>
<td>2.14</td>
<td>0.83</td>
<td>3.95</td>
<td>0.40</td>
<td>OH$^*$→H$_2$O</td>
</tr>
<tr>
<td>FeSe$_2$</td>
<td>1.39</td>
<td>0.22</td>
<td>3.36</td>
<td>1.01</td>
<td>OH$^*$→H$_2$O</td>
</tr>
<tr>
<td>FeTe$_2$</td>
<td>1.09</td>
<td>0.11</td>
<td>3.22</td>
<td>1.13</td>
<td>OH$^*$→H$_2$O</td>
</tr>
<tr>
<td>CoS$_2$</td>
<td>2.93</td>
<td>1.06</td>
<td>4.34</td>
<td>0.65</td>
<td>O$_2$→OOH$^*$</td>
</tr>
<tr>
<td>CoSe$_2$</td>
<td>2.53</td>
<td>0.86</td>
<td>4.12</td>
<td>0.43</td>
<td>O$_2$→OOH$^*$</td>
</tr>
<tr>
<td>CoTe$_2$</td>
<td>2.25</td>
<td>0.65</td>
<td>3.84</td>
<td>0.59</td>
<td>OH$^*$→H$_2$O</td>
</tr>
<tr>
<td>NiS$_2$</td>
<td>3.49</td>
<td>1.37</td>
<td>4.51</td>
<td>0.82</td>
<td>O$_2$→OOH$^*$</td>
</tr>
<tr>
<td>NiSe$_2$</td>
<td>3.13</td>
<td>1.18</td>
<td>4.27</td>
<td>0.58</td>
<td>O$_2$→OOH$^*$</td>
</tr>
<tr>
<td>NiTe$_2$</td>
<td>2.77</td>
<td>0.93</td>
<td>4.09</td>
<td>0.40</td>
<td>O$_2$→OOH$^*$</td>
</tr>
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</table>
Table S11. Summary of the calculated ORR and OER overpotentials and the corresponding potential limiting steps (PLS) with respect to different equilibrium potential ($U_{eq}$) (1.11 V of DFT level of theory and 1.23 V of experimental value).

<table>
<thead>
<tr>
<th>TMDs</th>
<th>$U_{eq} = 1.11$ V</th>
<th></th>
<th>$U_{eq} = 1.23$ V</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>ORR</td>
<td>OER</td>
<td>PLS</td>
<td>ORR</td>
</tr>
<tr>
<td>MnS$_2$</td>
<td>$\eta^{ORR}$</td>
<td>0.77</td>
<td>O$_2$→OOH*</td>
<td>0.82</td>
</tr>
<tr>
<td>MnSe$_2$</td>
<td>0.59</td>
<td>O$_2$→OOH*</td>
<td>0.89</td>
<td>OH*→O*</td>
</tr>
<tr>
<td>MnTe$_2$</td>
<td>0.67</td>
<td>OH*→H$_2$O</td>
<td>0.80</td>
<td>OH*→O*</td>
</tr>
<tr>
<td>FeS$_2$</td>
<td>0.62</td>
<td>OH*→H$_2$O</td>
<td>0.69</td>
<td>O*→OOH*</td>
</tr>
<tr>
<td>FeSe$_2$</td>
<td>0.89</td>
<td>OH*→H$_2$O</td>
<td>0.86</td>
<td>O*→OOH*</td>
</tr>
<tr>
<td>FeTe$_2$</td>
<td>1.01</td>
<td>OH*→H$_2$O</td>
<td>1.02</td>
<td>O*→OOH*</td>
</tr>
<tr>
<td>CoS$_2$</td>
<td>1.01</td>
<td>O$_2$→OOH*</td>
<td>0.76</td>
<td>OH*→O*</td>
</tr>
<tr>
<td>CoSe$_2$</td>
<td>0.79</td>
<td>O$_2$→OOH*</td>
<td>0.55</td>
<td>OH*→O*</td>
</tr>
<tr>
<td>CoTe$_2$</td>
<td>0.51</td>
<td>OH*→H$_2$O</td>
<td>0.50</td>
<td>OH*→O*</td>
</tr>
<tr>
<td>NiS$_2$</td>
<td>1.18</td>
<td>O$_2$→OOH*</td>
<td>1.00</td>
<td>OH*→O*</td>
</tr>
<tr>
<td>NiSe$_2$</td>
<td>0.94</td>
<td>O$_2$→OOH*</td>
<td>0.83</td>
<td>OH*→O*</td>
</tr>
<tr>
<td>NiTe$_2$</td>
<td>0.76</td>
<td>O$_2$→OOH*</td>
<td>0.73</td>
<td>OH*→O*</td>
</tr>
</tbody>
</table>

Table S12. The experimentally measured overpotentials of ORR and OER in an alkaline media.

<table>
<thead>
<tr>
<th>Materials</th>
<th>$\eta^{ORR}$ (mV)</th>
<th>$\eta^{OER}$ (mV)</th>
<th>ref</th>
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<tbody>
<tr>
<td>CoSe$_2$/Se-rGO</td>
<td>327</td>
<td>5</td>
<td></td>
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<tr>
<td>Co@DNC@FeSe$_2$-0.5</td>
<td>288</td>
<td>42</td>
<td></td>
</tr>
<tr>
<td>CoO-CoSe$_2$@N-CNTs/rGO</td>
<td>250</td>
<td>43</td>
<td></td>
</tr>
<tr>
<td>Co@CoTe$_2$</td>
<td>284</td>
<td>6</td>
<td></td>
</tr>
<tr>
<td>Fe, Ni-CoS$_2$/GC</td>
<td>242</td>
<td>44</td>
<td></td>
</tr>
<tr>
<td>NiTe$_2$ nanosheet</td>
<td>310</td>
<td>45</td>
<td></td>
</tr>
<tr>
<td>FeS$_2$@CoS$_2$</td>
<td>302</td>
<td>46</td>
<td></td>
</tr>
<tr>
<td>NiSe$_2$/g-C$_3$N$_4$/NF</td>
<td>290</td>
<td>47</td>
<td></td>
</tr>
<tr>
<td>Fe-CoS$_2$/CoS$_2$@NC</td>
<td>300</td>
<td>48</td>
<td></td>
</tr>
<tr>
<td>FeSe$_2$@CoSe$_2$/rGO-2</td>
<td>260</td>
<td>49</td>
<td></td>
</tr>
</tbody>
</table>
References


42. Liu, M.; Zhang, M.; Zhang, P.; Xing, Z.; Jiang, B.; Yu, Y.; Cai, Z.; Li, J.; Zou, J., ZIF-67-derived dodecahedral Co@N-doped graphitized carbon protected by a porous FeS2 thin-layer as an efficient catalyst to promote the oxygen reduction reaction. ACS Sustain. Chem. Eng. 2020, 8 (10), 4194-4206.
49. Zhu, G.; Xie, X.; Li, X.; Liu, Y.; Shen, X.; Xu, K.; Chen, S., Nanocomposites based on CoSe2-decorated FeSe2 nanoparticles supported on reduced graphene oxide as...