

## Supporting Information

### **Size-Dependent Electrocatalytic Activity of ORR/OER on Palladium Nanoclusters**

### **Anchored Defective MoS<sub>2</sub> Monolayers**

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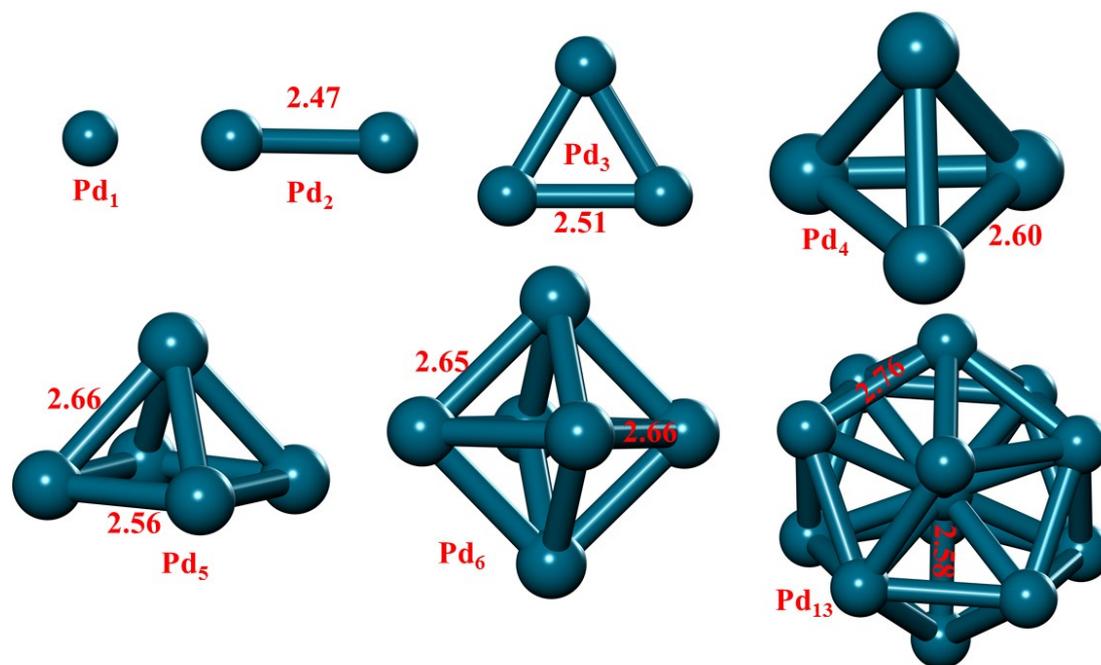
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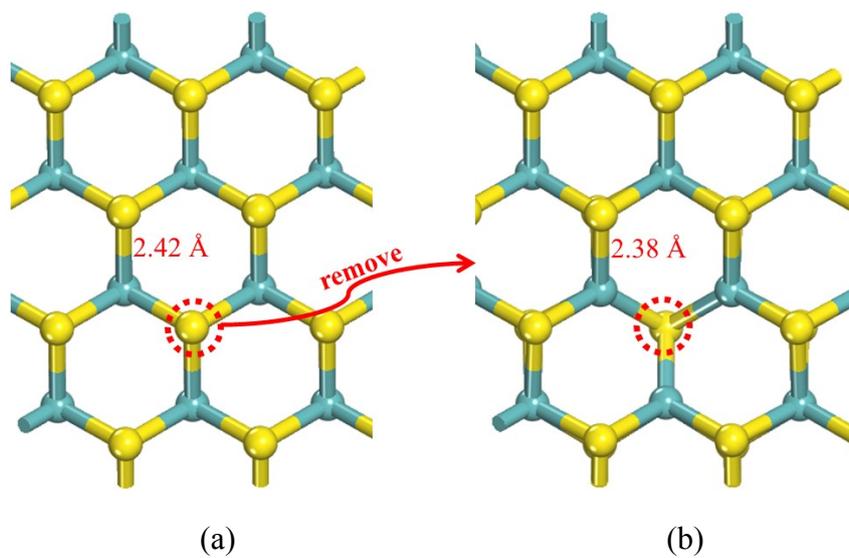
xjz\_hmily@163.com or zhaojingxiang@hrbnu.edu.cn (JZ)

**Table S1:** The computed binding energies per Pd atom ( $E_b$ , eV) for Pd<sub>13</sub> cluster on defective MoS<sub>2</sub> monolayer with different supercells.

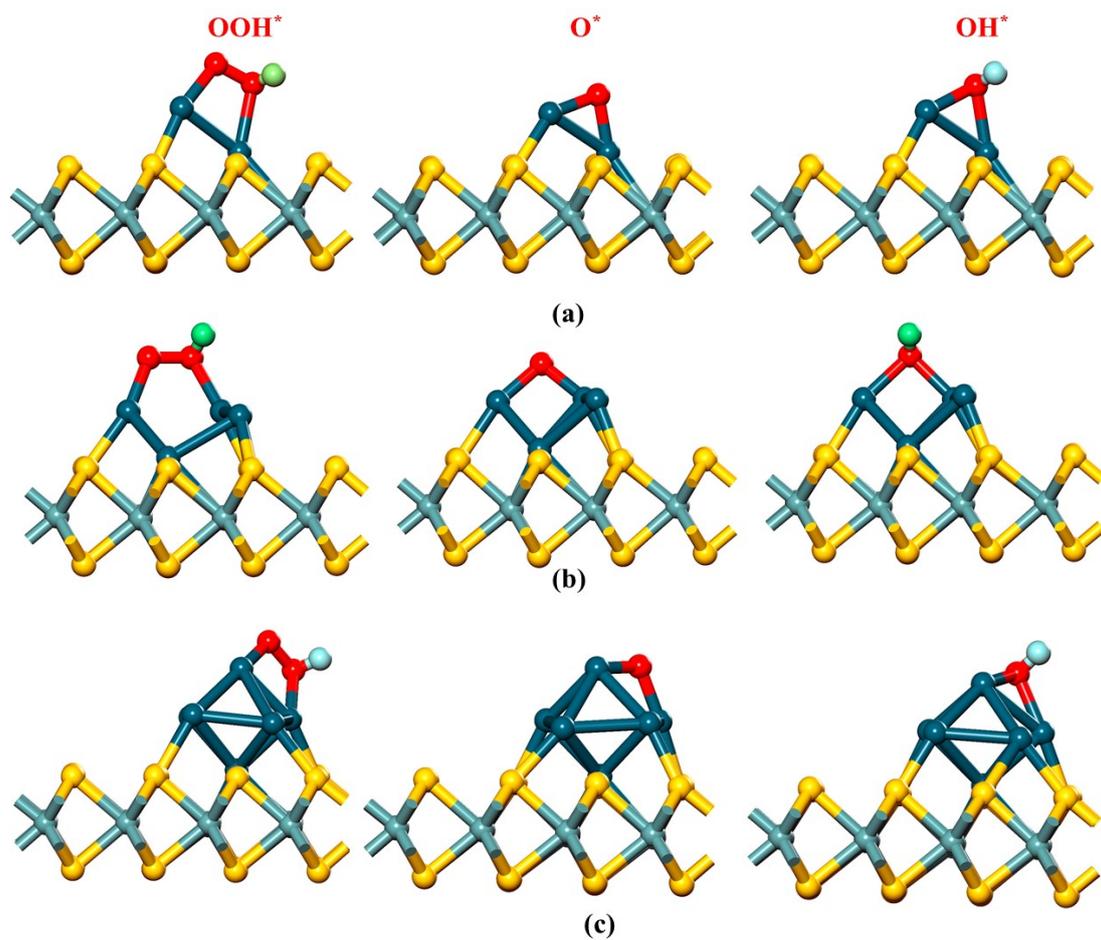
supercell	4×4	5×5	6×6
$E_b$	-3.16	-3.18	-3.18



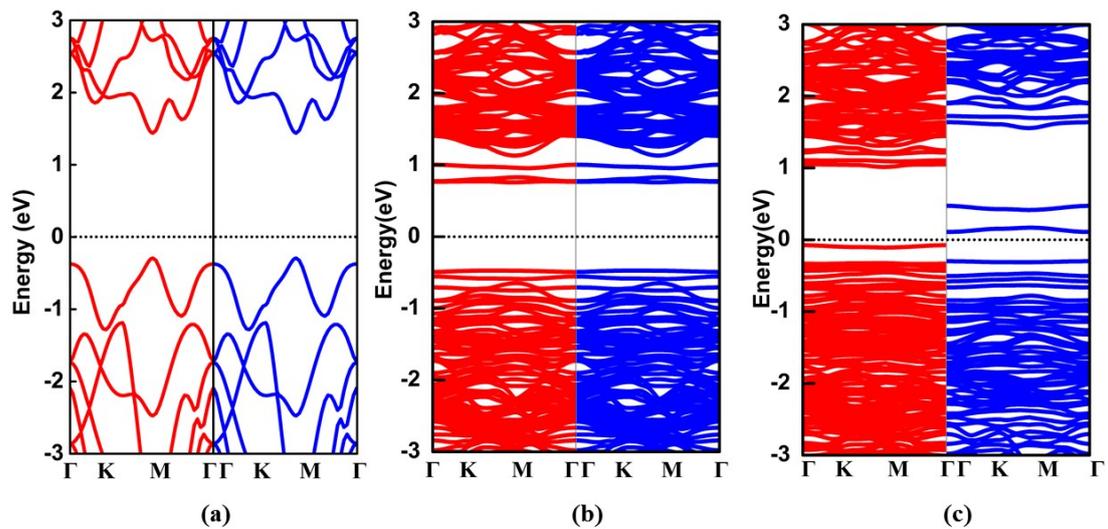
**Fig. S1.** The optimized stable structures of various Pd<sub>n</sub> clusters (n = 1~6, and 13) and the key Pd-Pd bond lengths.



**Fig. S2.** The optimized structures of (a) pristine and (b) defective MoS<sub>2</sub> monolayers.



**Fig. S3.** The optimized adsorption configurations of OOH\*, O\*, and OH\* intermediates on (a) Pd<sub>2</sub>/MoS<sub>2</sub>, (b) Pd<sub>4</sub>/MoS<sub>2</sub>, and (c) Pd<sub>6</sub>/MoS<sub>2</sub> catalysts.



**Fig. S4.** The computed band structures of (a) pristine MoS<sub>2</sub> monolayer, (b) Pd<sub>2</sub>/MoS<sub>2</sub>, and (c) Pd<sub>6</sub>/MoS<sub>2</sub>. The Fermi level was set to zero in black dotted line.