

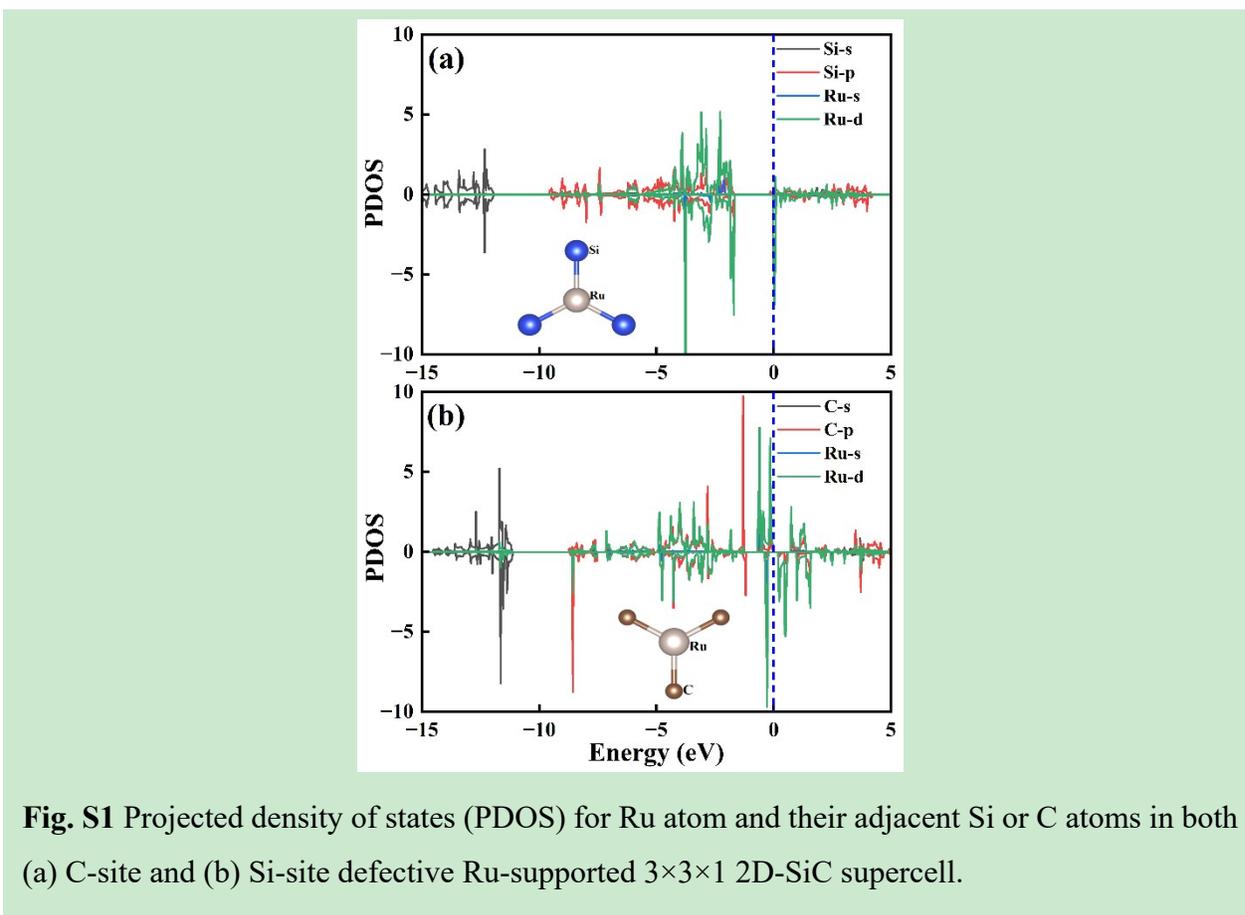
### Electronic Supplementary Information

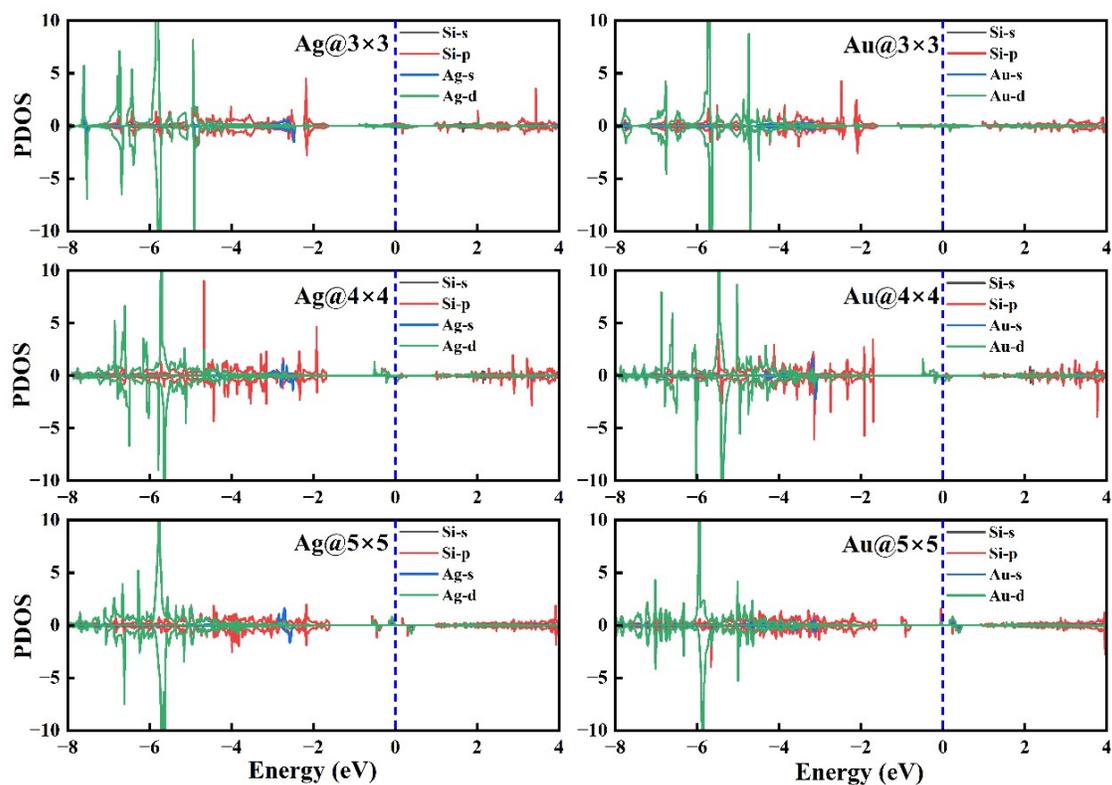
## Modulating the Electronic Properties and Hydrogen Evolution Reaction Performance of Precious-Metal on 2D-SiC via Surface Defect

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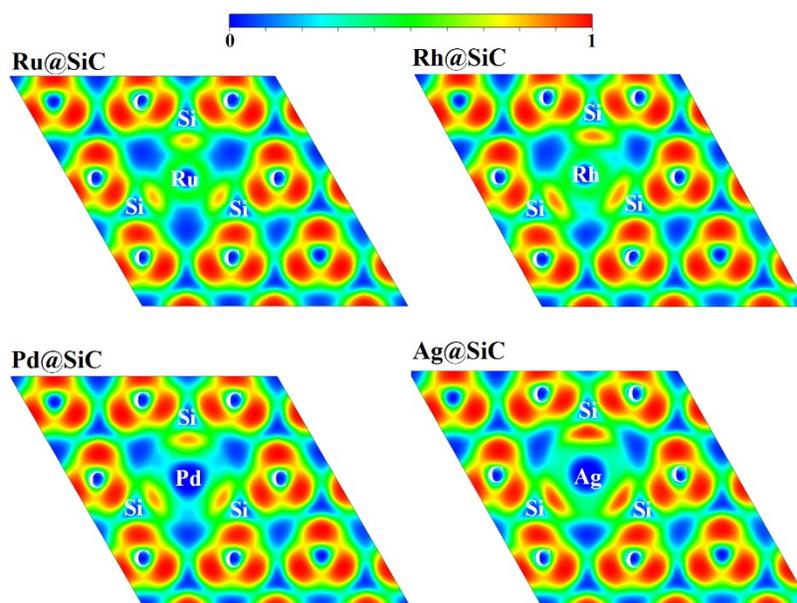
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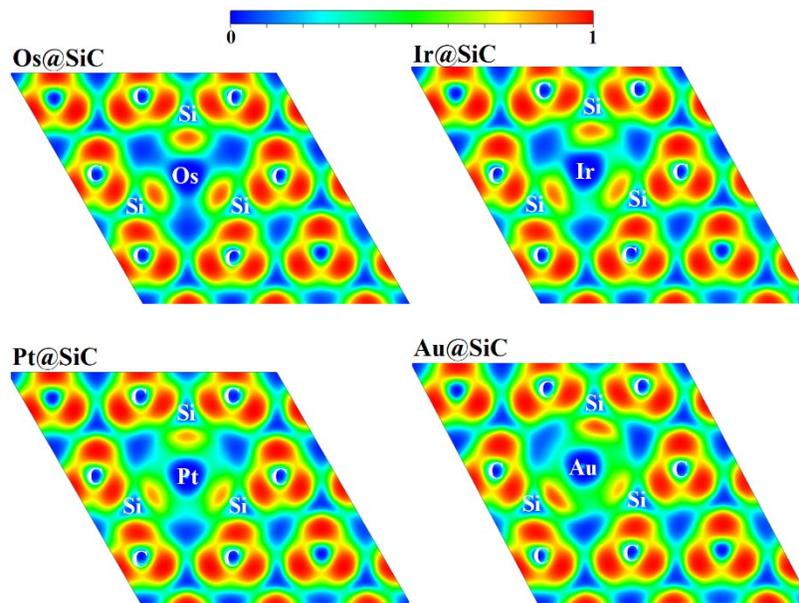




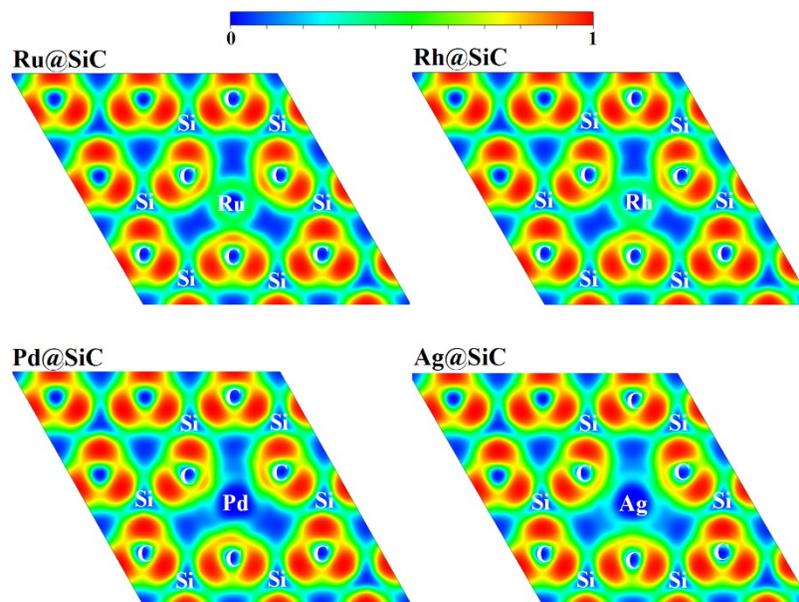
**Fig. S2** PDOS of PM atom and Si atoms adjacent to the PM in C-site defect supported Ag and Au.



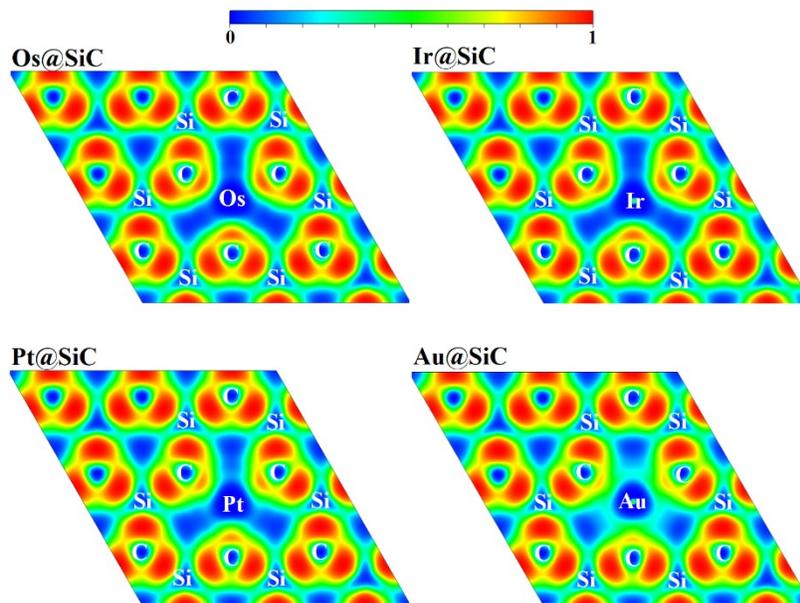
**Fig. S3.** Planar projection maps of the electron localization function for Ru-, Rh-, Pd-, and Ag-supported C-site defect in  $3 \times 3 \times 1$  2D-SiC supercell.



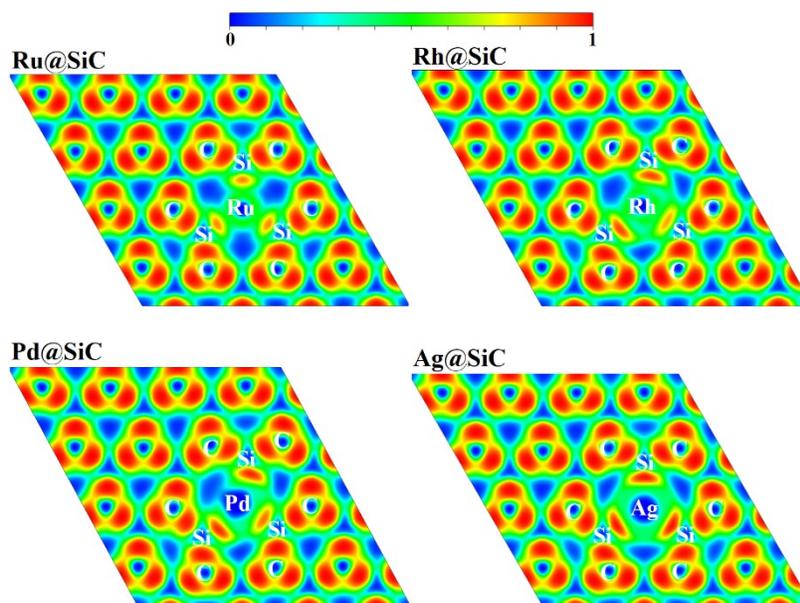
**Fig. S4.** Planar projection maps of the electron localization function for Os-, Ir-, Pt-, and Au-supported C-site defect in  $3\times 3\times 1$  2D-SiC supercell.



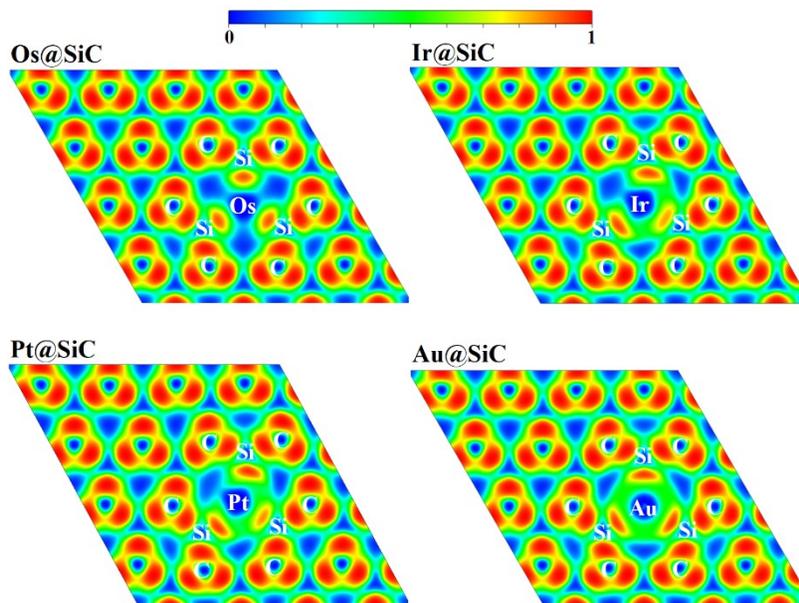
**Fig. S5.** Planar projection maps of the electron localization function for Ru-, Rh-, Pd-, and Ag-supported Si-site defect in  $3\times 3\times 1$  2D-SiC supercell.



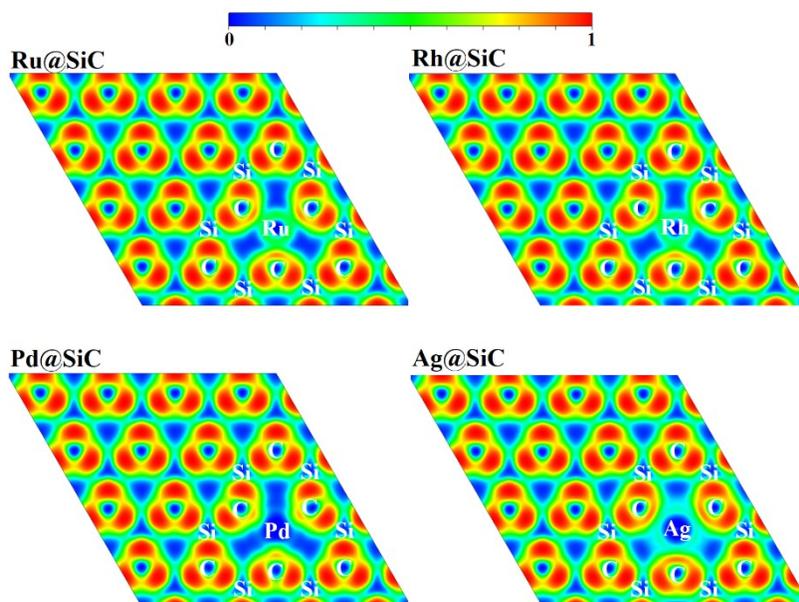
**Fig. S6.** Planar projection maps of the electron localization function for Os-, Ir-, Pt-, and Au-supported Si-site defect in  $3\times 3\times 1$  2D-SiC supercell.



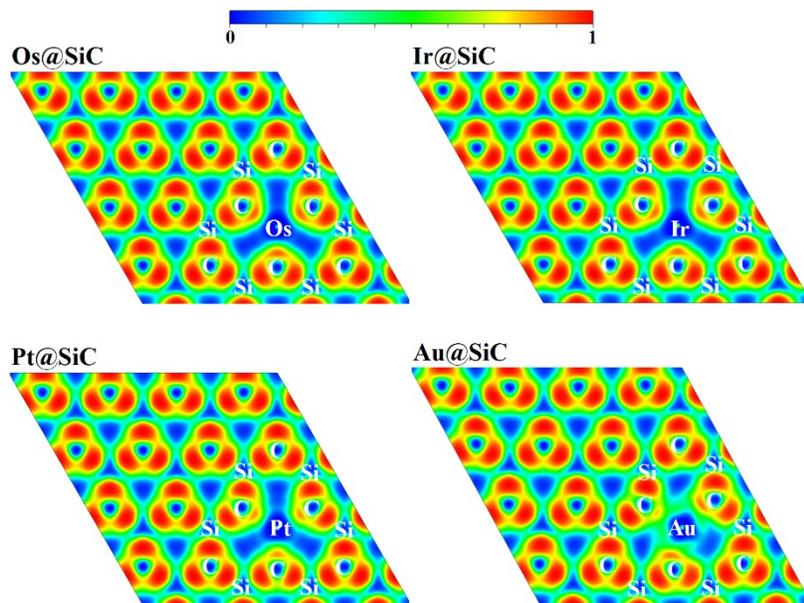
**Fig. S7.** Planar projection maps of the electron localization function for Ru-, Rh-, Pd-, and Ag-supported C-site defect in  $3\times 3\times 1$  2D-SiC supercell.



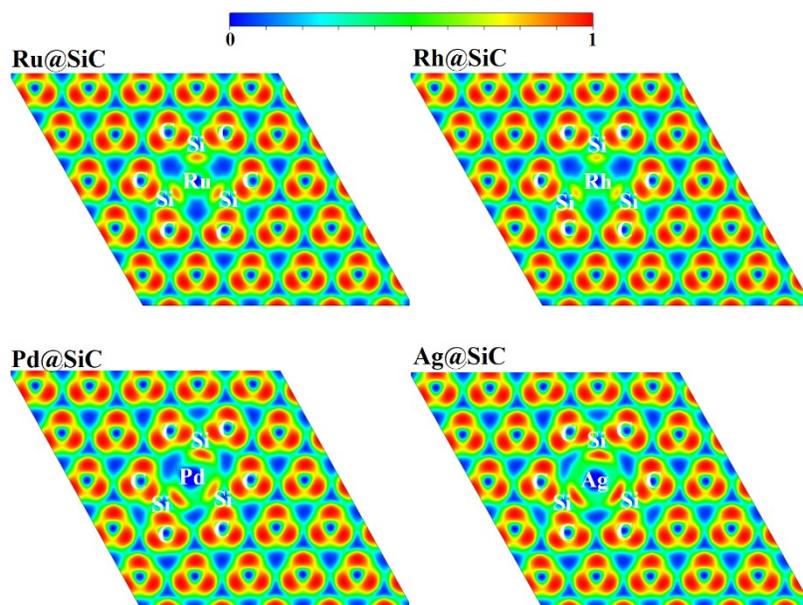
**Fig. S8.** Planar projection maps of the electron localization function for Os-, Ir-, Pt-, and Au-supported C-site defect in  $4\times 4\times 1$  2D-SiC supercell.



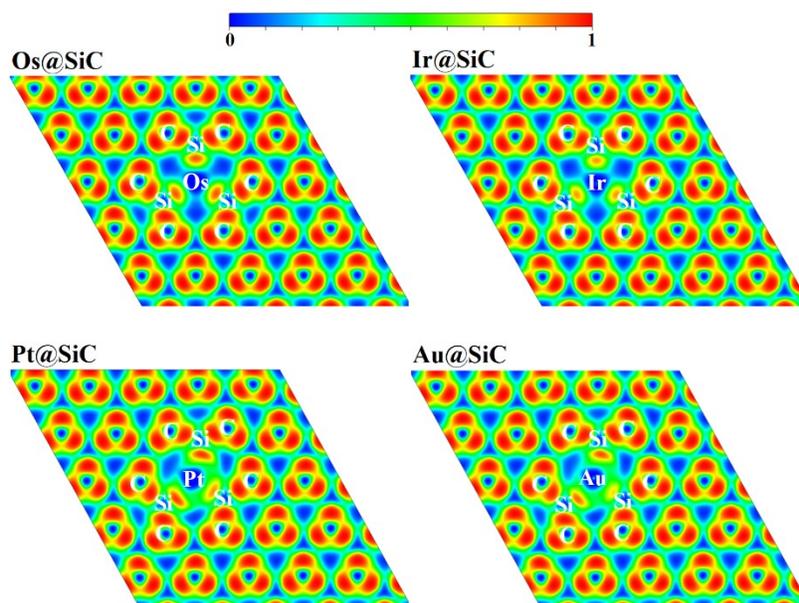
**Fig. S9.** Planar projection maps of the electron localization function for Ru-, Rh-, Pd-, and Ag-supported Si-site defect in  $4\times 4\times 1$  2D-SiC supercell.



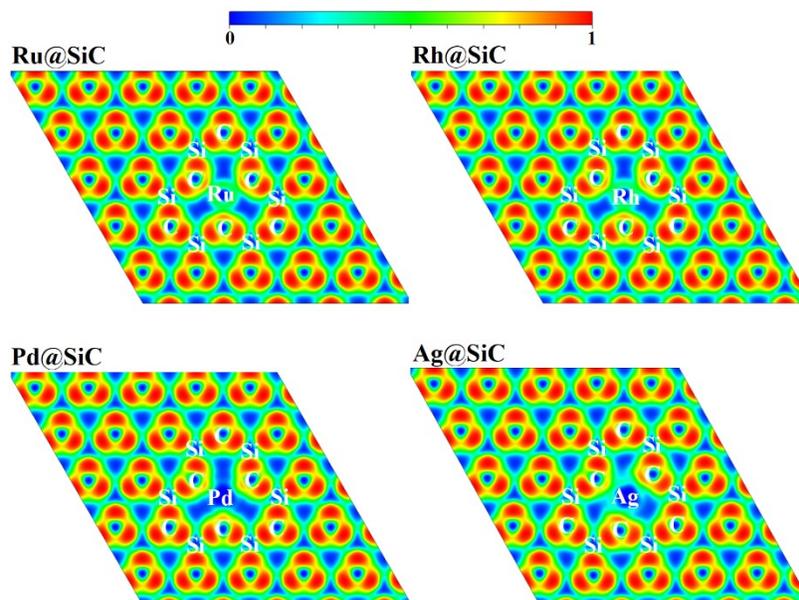
**Fig. S10.** Planar projection maps of the electron localization function for Os-, Ir-, Pt-, and Au-supported Si-site defect in  $4 \times 4 \times 1$  2D-SiC supercell.



**Fig. S11.** Planar projection maps of the electron localization function for Ru-, Rh-, Pd-, and Ag-supported C-site defect in  $5 \times 5 \times 1$  2D-SiC supercell.

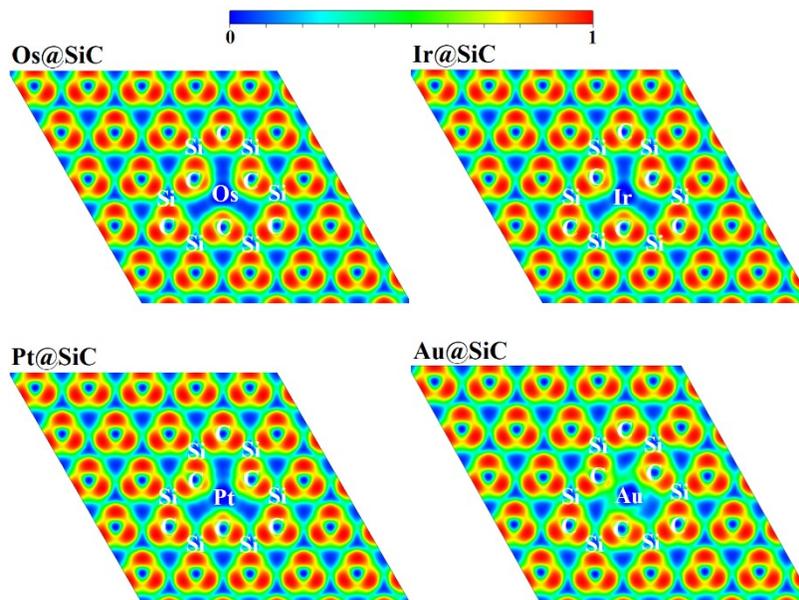


**Fig. S12.** Planar projection maps of the electron localization function for Os-, Ir-, Pt-, and Au-supported C-site defect in  $5 \times 5 \times 1$  2D-SiC supercell.

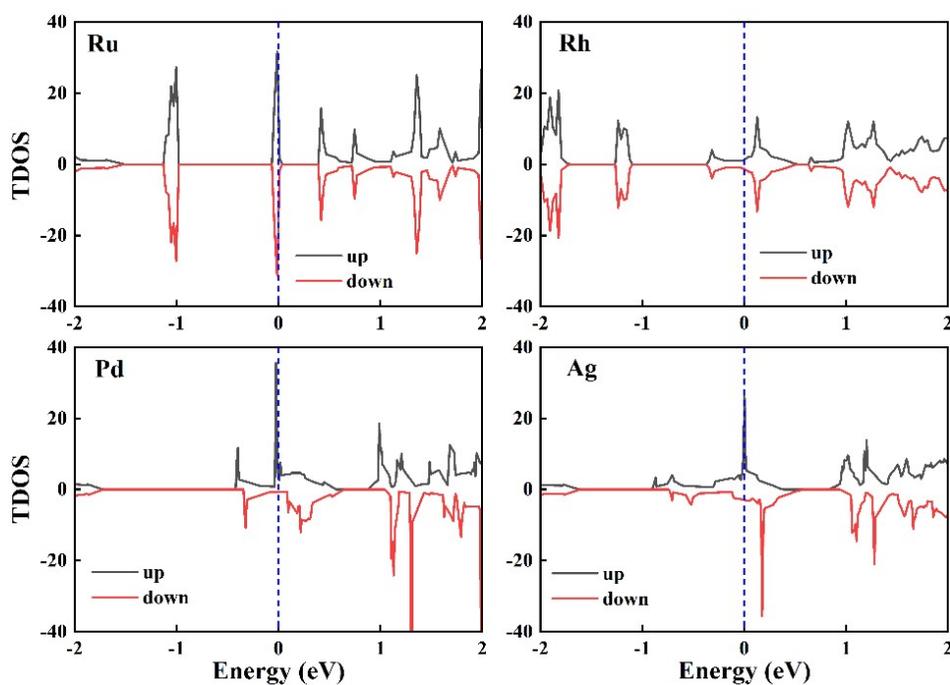


**Fig. S13.** Planar projection maps of the electron localization function for Ru-, Rh-, Pd-, and Ag-supported Si-site defect in  $5 \times 5 \times 1$  2D-SiC supercell.

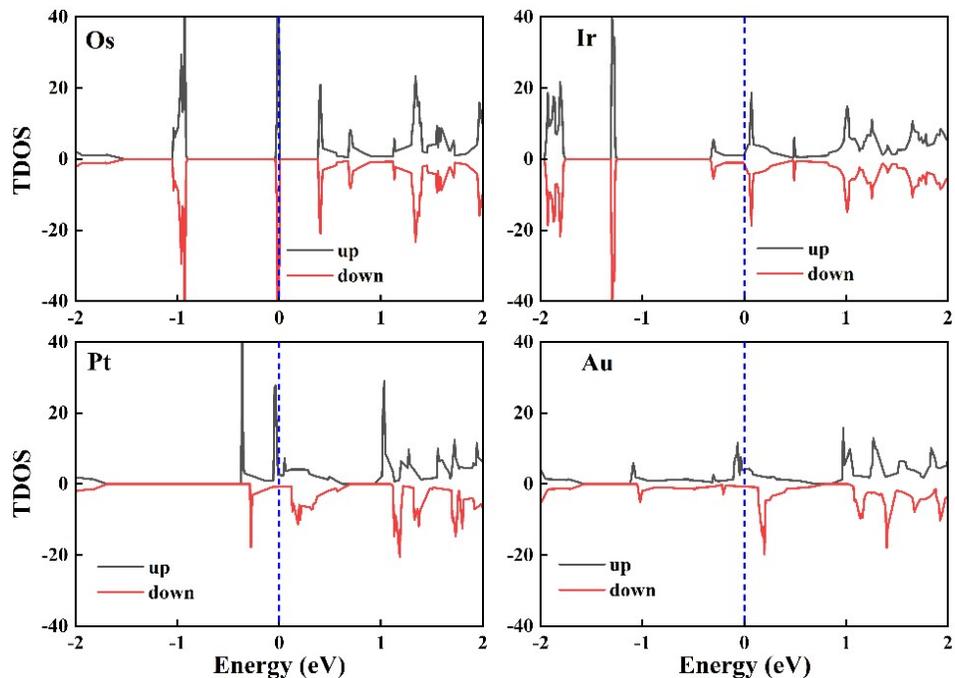




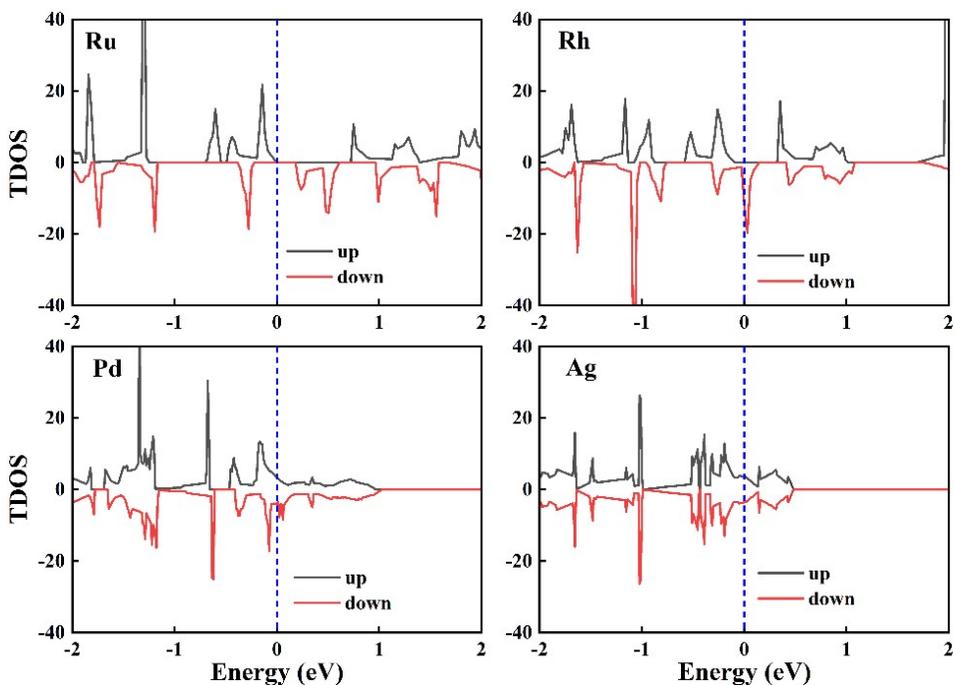
**Fig. S14.** Planar projection maps of the electron localization function for Os-, Ir-, Pt-, and Au-supported Si-site defect in  $5 \times 5 \times 1$  2D-SiC supercell.



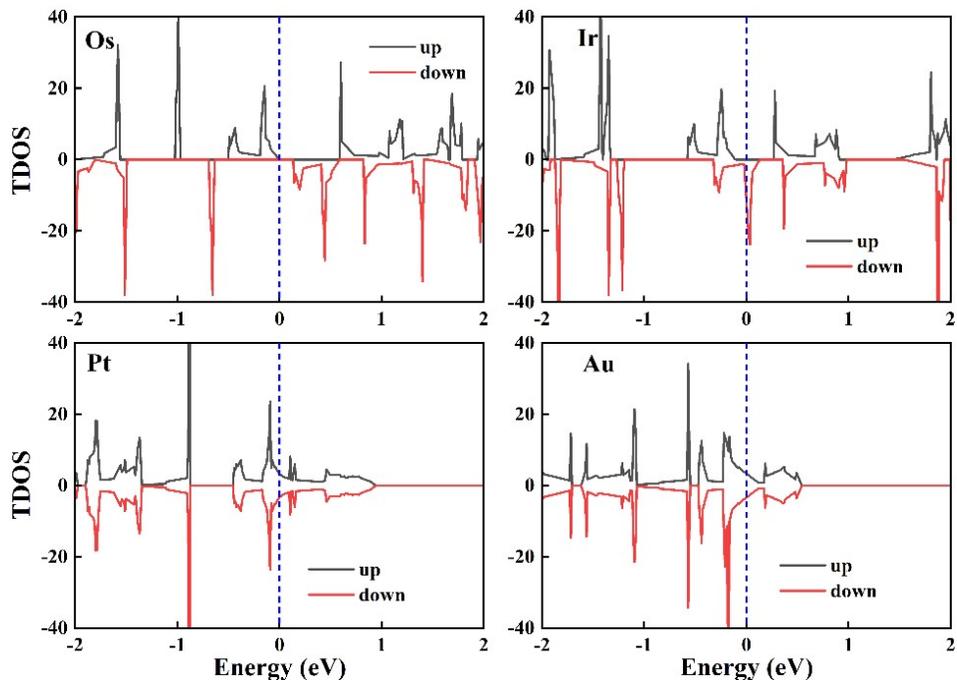
**Fig. S15.** TDOS for Ru, Rh, Pd, and Ag-supported on the C-site defect in  $3 \times 3 \times 1$  2D-SiC supercell.



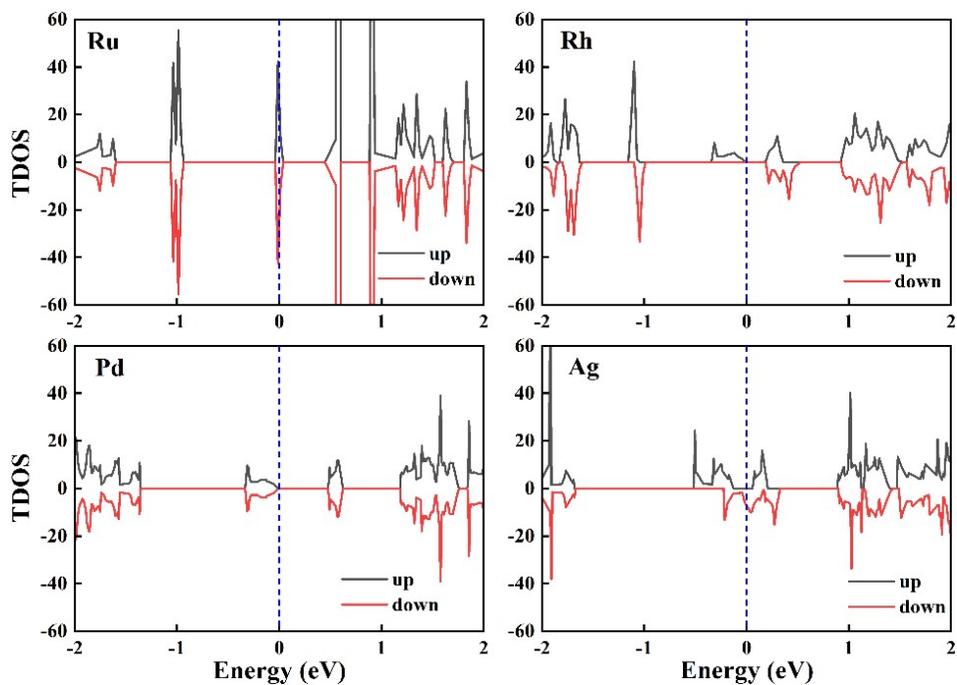
**Fig. S16.** TDOS for Os, Ir, Pt, and Au-supported on the C-site defect in  $3 \times 3 \times 1$  2D-SiC supercell.



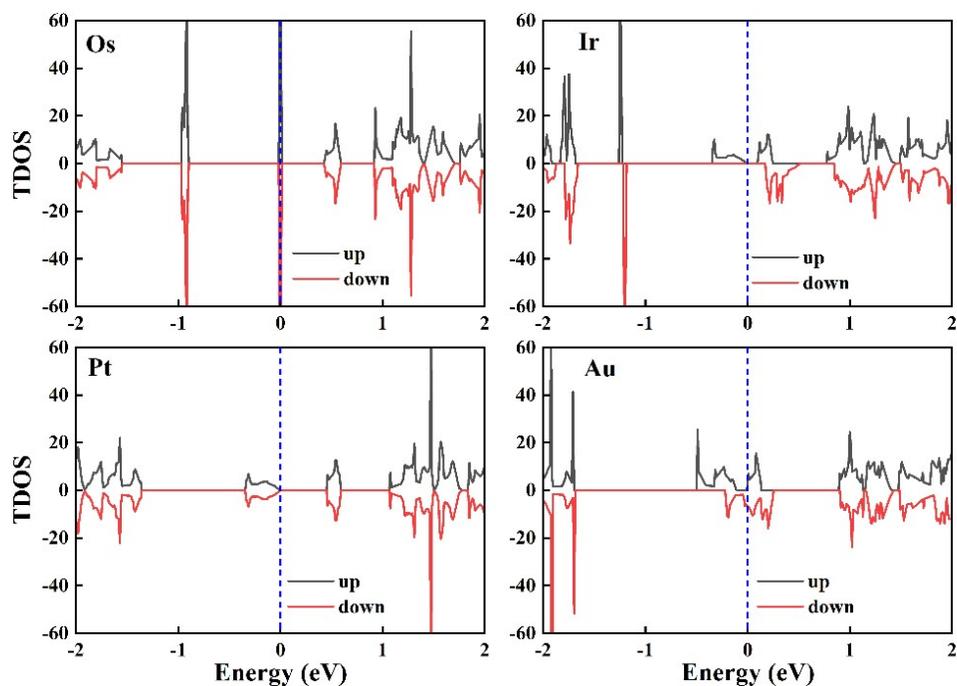
**Fig. S17.** TDOS for Ru, Rh, Pd, and Ag-supported on the Si-site defect in  $3 \times 3 \times 1$  2D-SiC supercell.



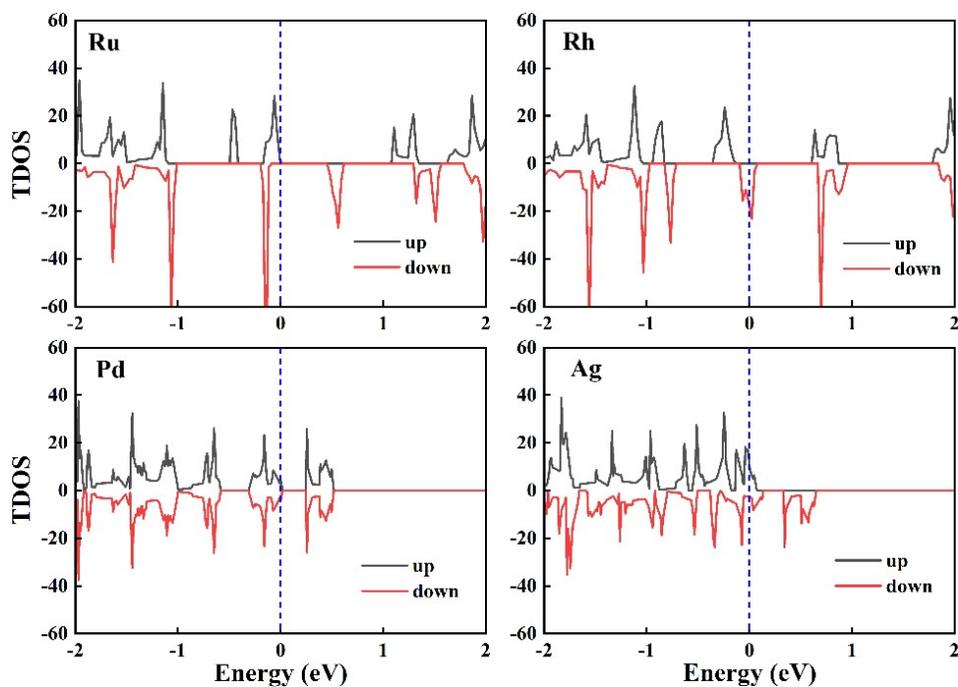
**Fig. S18.** TDOS for Os, Ir, Pt, and Au-supported on the Si-site defect in  $3\times 3\times 1$  2D-SiC supercell.



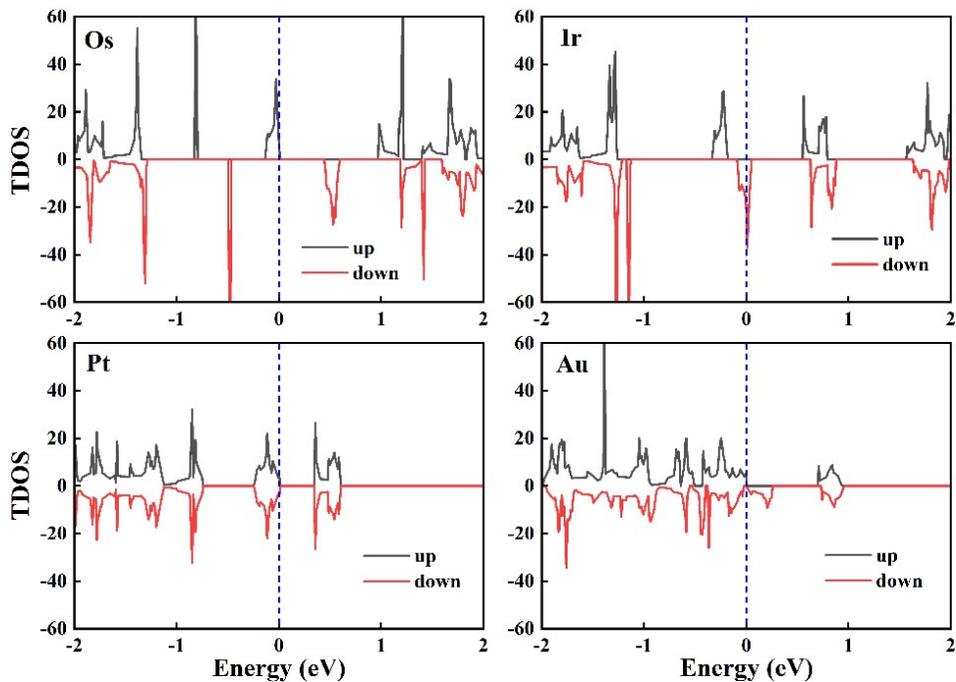
**Fig. S19.** TDOS for Ru, Rh, Pd, and Ag-supported on the C-site defect in  $4\times 4\times 1$  2D-SiC supercell.



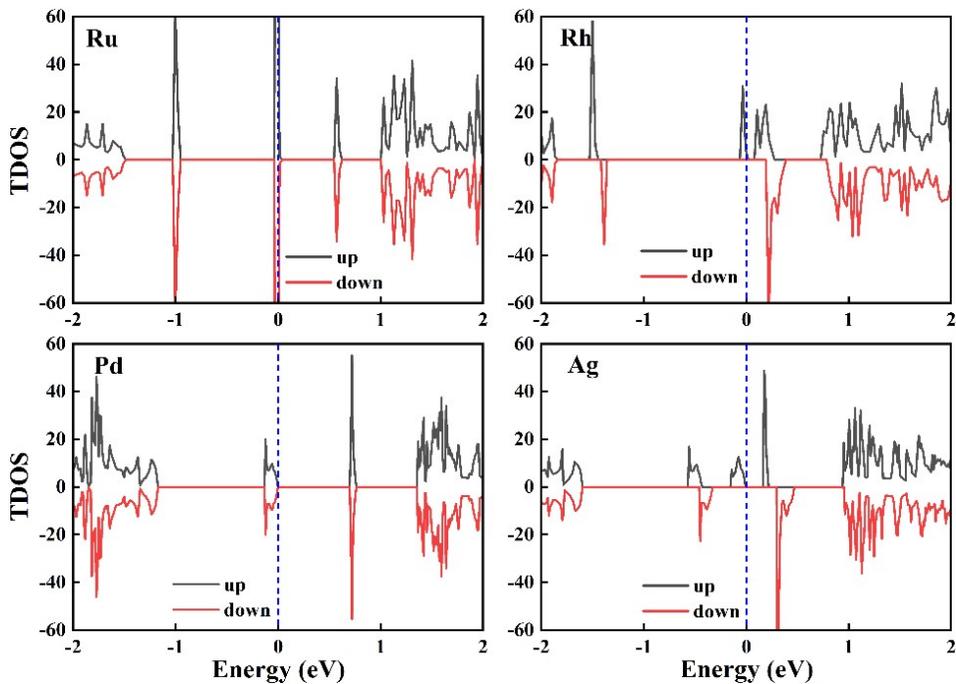
**Fig. S20.** TDOS for Os, Ir, Pt, and Au-supported on the C-site defect in  $4 \times 4 \times 1$  2D-SiC supercell.



**Fig. S21.** TDOS for Ru, Rh, Pd, and Ag-supported on the Si-site defect in  $4 \times 4 \times 1$  2D-SiC supercell.



**Fig. S22.** TDOS for Os, Ir, Pt, and Au-supported on the Si-site defect in  $4 \times 4 \times 1$  2D-SiC supercell.



**Fig. S23.** TDOS for Ru, Rh, Pd, and Ag-supported on the C-site defect in  $5 \times 5 \times 1$  2D-SiC supercell.

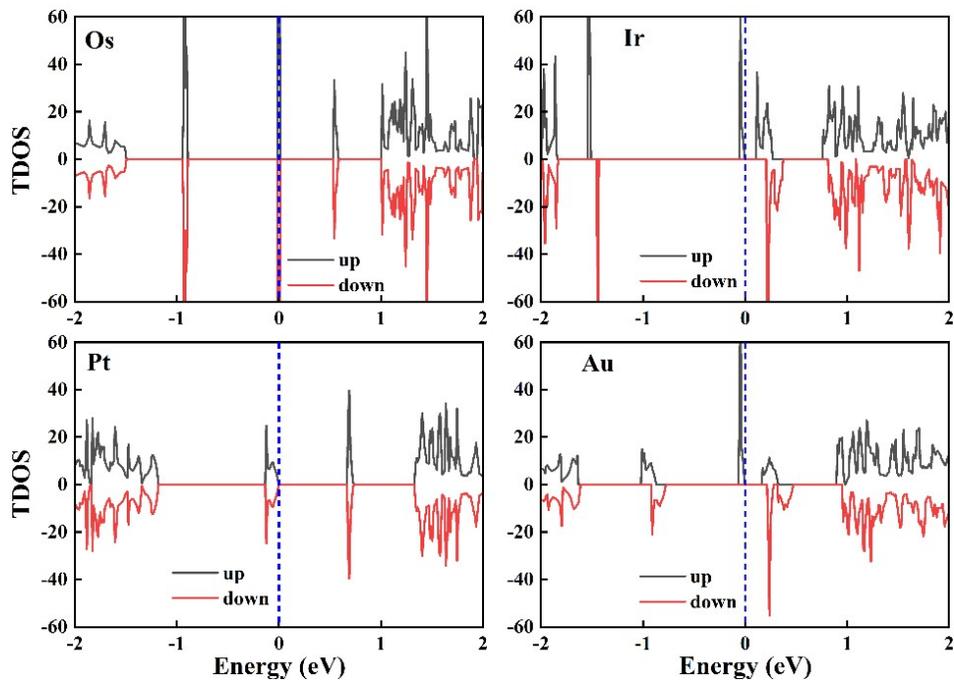


Fig. S24. TDOS for Os, Ir, Pt, and Au-supported on the C-site defect in  $5 \times 5 \times 1$  2D-SiC supercell.

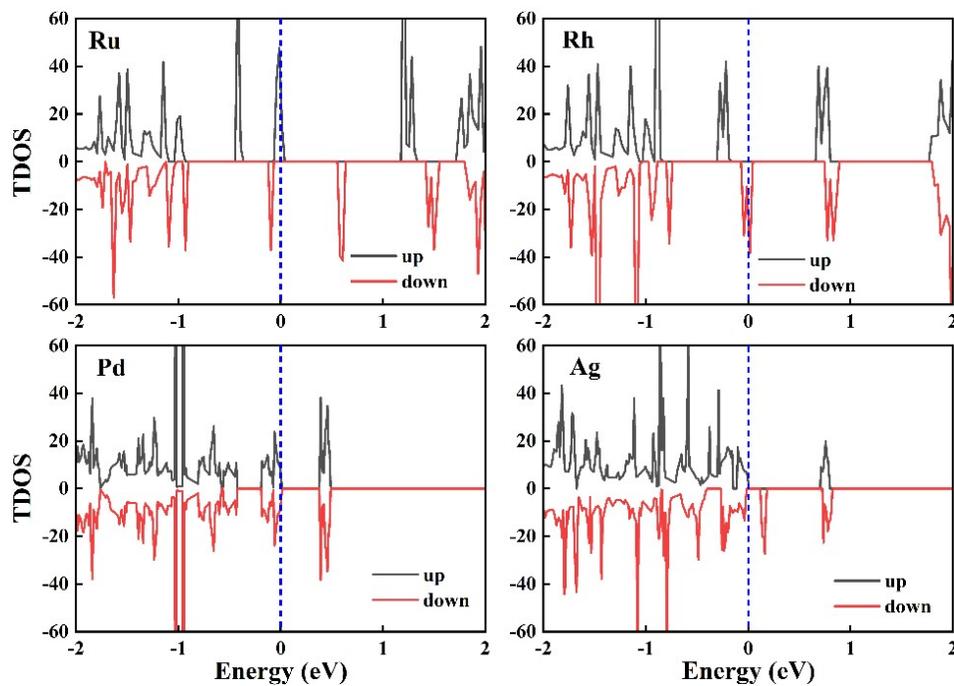
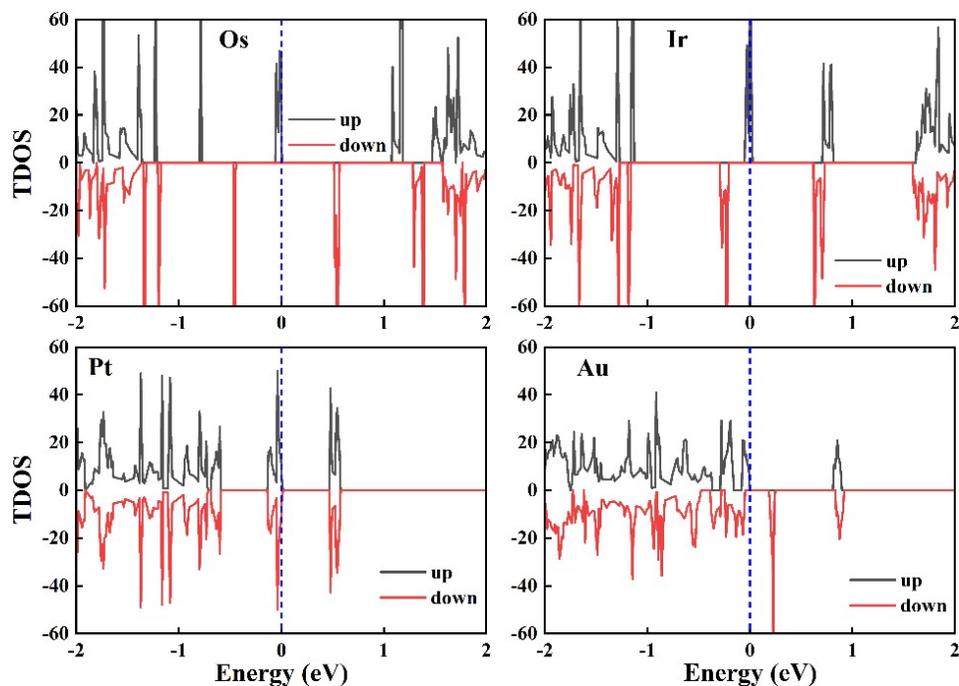


Fig. S25. TDOS for Ru, Rh, Pd, and Ag-supported on the Si-site defect in  $5 \times 5 \times 1$  2D-SiC supercell.



**Fig. S26.** TDOS for Os, Ir, Pt, and Au-supported on the Si-site defect in  $5 \times 5 \times 1$  2D-SiC supercell.

### Structural information of the primitive unit cell of 2D-SiC.

The detailed structural parameters of the primitive 2D-SiC can be found in Reference [Nanomaterials 2021, 11, 1799. <https://doi.org/10.3390/nano11071799>].