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Unveiling the HER Potential of TM-Substituted $PdTe_2$ Monolayers: A First-Principles Study

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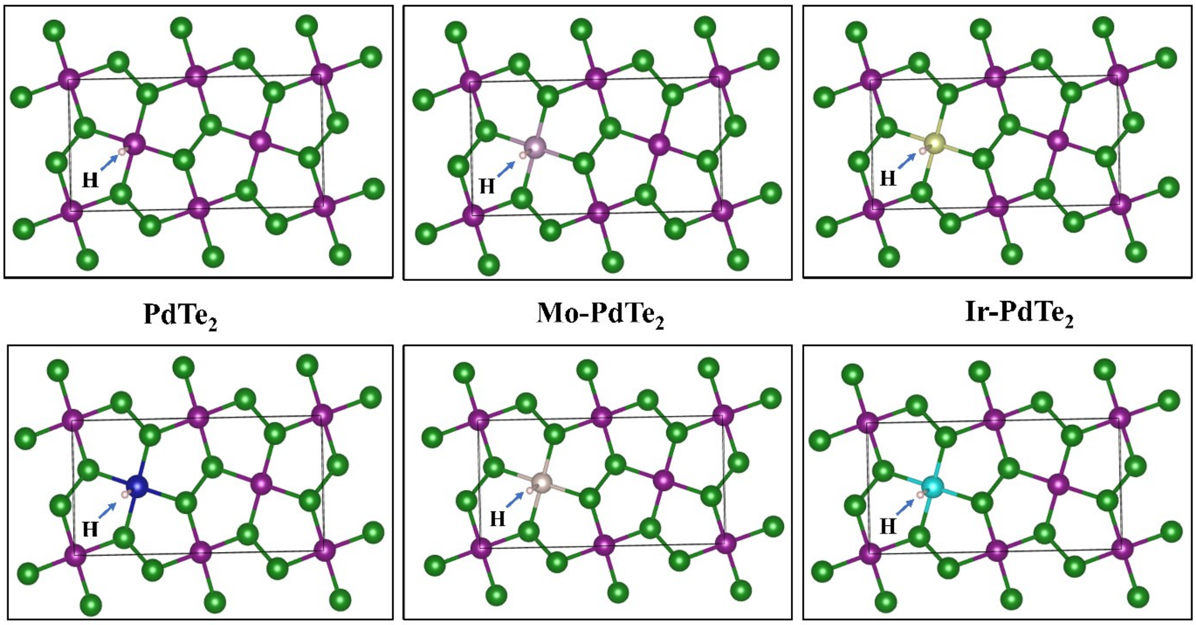

$PdTe_2$ **Mo-$PdTe_2$** **Ir-$PdTe_2$**

Cr-$PdTe_2$ **Ru-$PdTe_2$** **Ti-$PdTe_2$**

Figure S1: Optimized Geometry of H-adsorbed $PdTe_2$ and its derivatives.

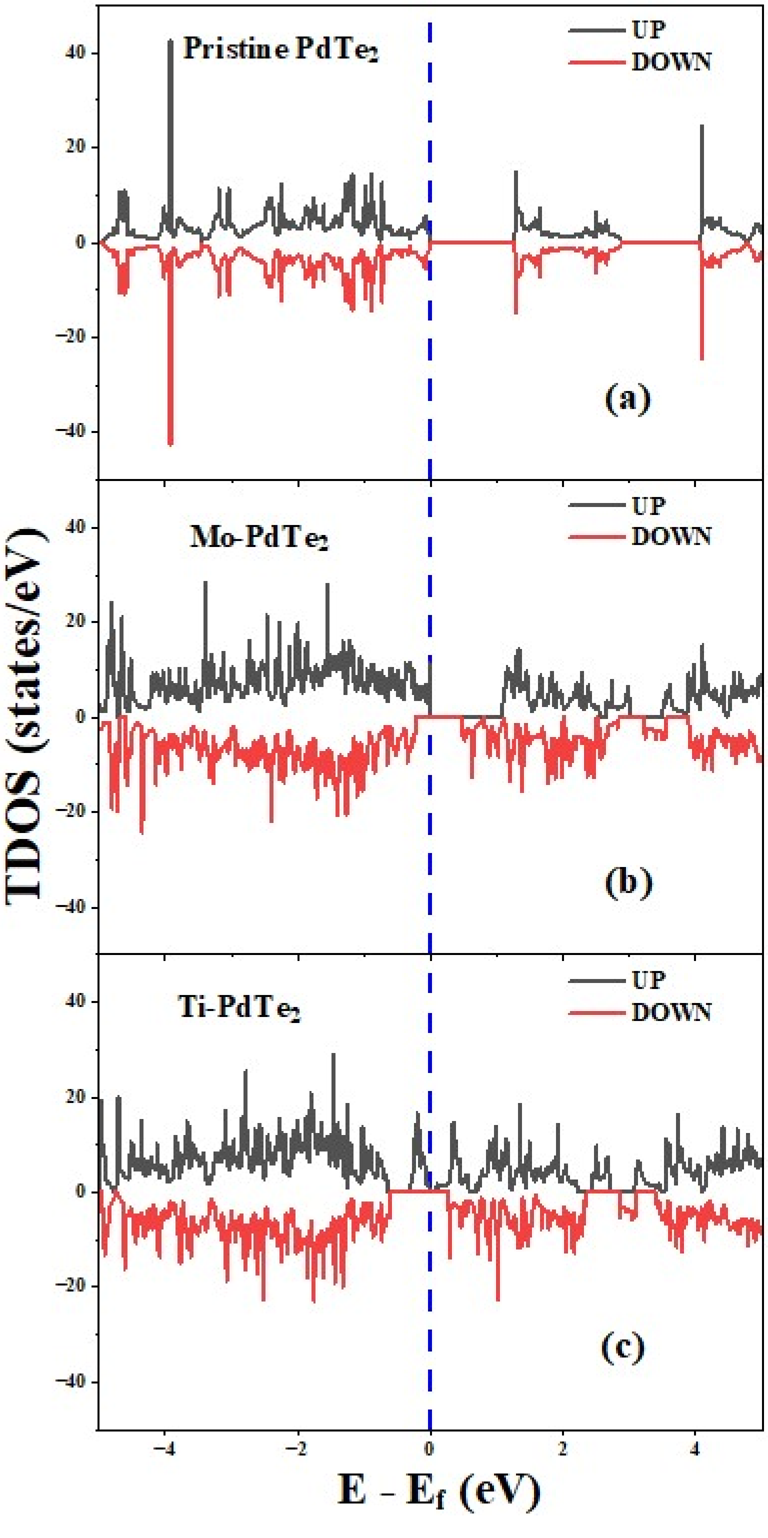

Figure S2: TDOS of pristine $PdTe_2$ and metal substituted $PdTe_2$ systems. (a) Pristine $PdTe_2$ (b) Mo-doped $PdTe_2$ (c) Ti-doped $PdTe_2$. The spin-up and spin-down channels are shown for each system. The Fermi level is set to 0 eV (indicated by the blue dashed line). Doping significantly modifies the electronic structure, particularly near the Fermi level, indicating potential changes in electronic and catalytic properties.

Table S1. Formation energy per atom for pristine and transition-metal-doped $PdTe_2$ monolayers.

System	Formation Energy (eV)
$PdTe_2$	-0.72
Mo	2.40
Ti	0.43
Cr	3.23
Ir	-0.82
Ru	-0.50

Table S2. Adsorption energy and overpotential for hydrogen atom adsorbed at different positions (A–E) on the pristine $PdTe_2$ surface**.**

Position of H atom	Adsorption energy (eV)	Overpotential (V)
A	1.14	1.38
B	1.14	1.38
C	1.14	1.38
D	1.14	1.38
E	1.14	1.38

Table S3. Effect of Hubbard U on HER activity of doped $PdTe_2$.

System	U parameter	Overpotential (V)	Adsorption Energy (eV)
Mo-$PdTe_2$	0	-0.05	-0.29
	1	-0.08	-0.32
	2	-0.11	-0.35