Electtronic Supplementary Information

Effects of adatom and gas molecule adsorption on physical properties of tellurene: a first principles investigation

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S1. Top and side views of optimized adatoms adsorption structures (α, and β tellurene phases)

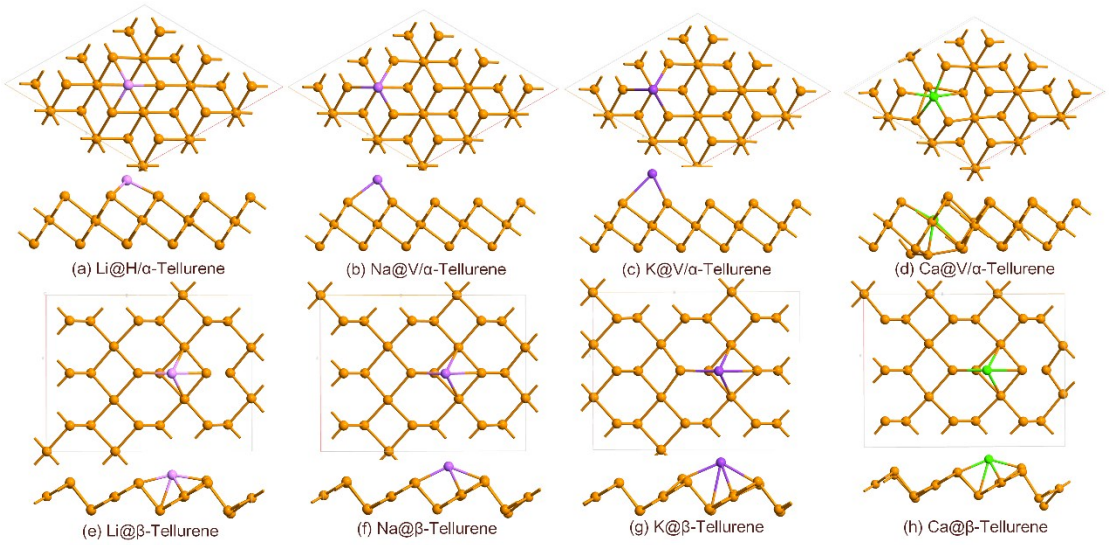

Figure S1. Top and side views of optimized alkali and alkaline-earth adatom (Li, Na, K, and Ca) adsorption structures (α, and β tellurene phases). The Te atoms are shown by orange balls, and adatoms are shown by balls with other different colors.

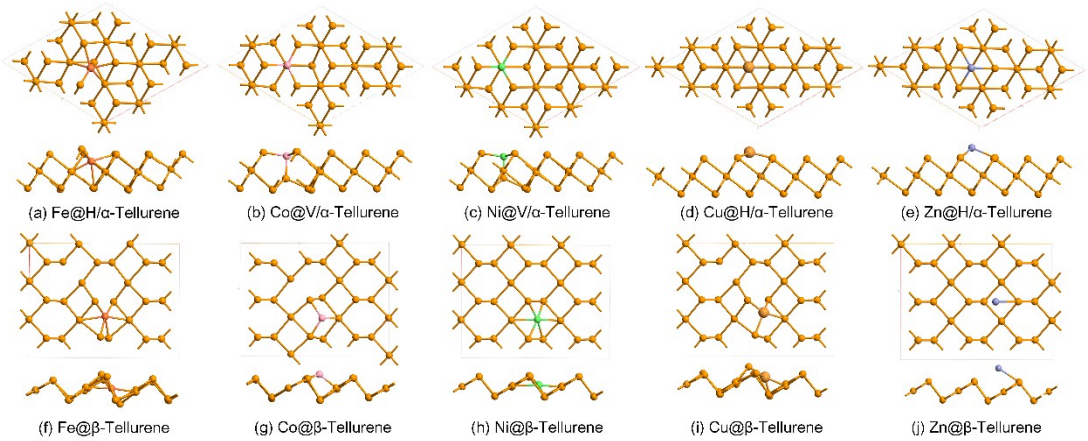

Figure. S1 Top and side views of optimized transition metal adatom (Fe, Co, Ni, Cu, and Zn) adsorption structures (α, and β tellurene phases). The Te atoms are shown by orange balls, and adatoms are shown by balls with other different colors.

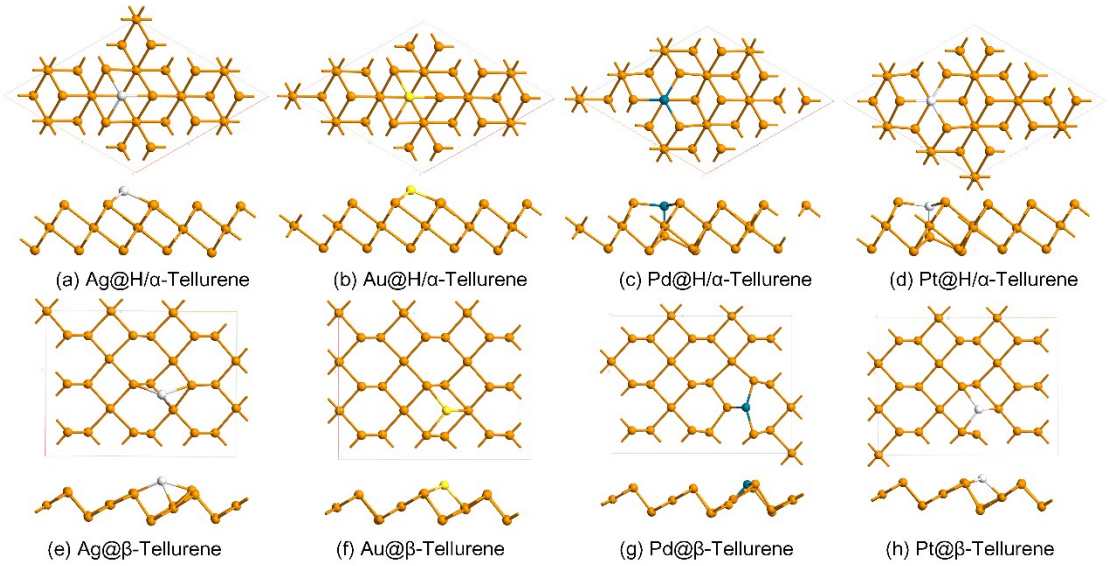

Figure. S1 Top and side views of optimized noble metal adatom (Ag, Au, Pd, and Pt) adsorption structures (α, and β tellurene phases). The Te atoms are shown by orange balls, and adatoms are shown by balls with other different colors.

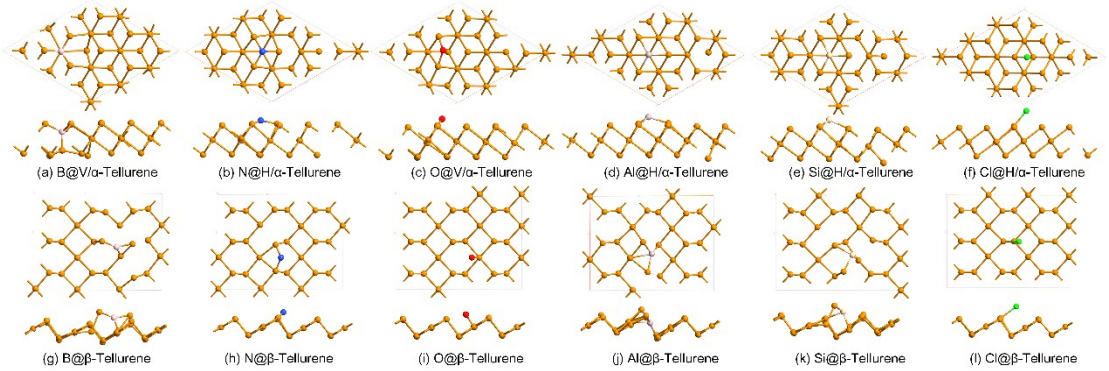

Figure. S1 Top and side views of optimized nometallic adatom (B, N, O, Si, and Cl), and Al adatom adsorption structures (α, and β tellurene phases). The Te atoms are shown by orange balls, and adatoms are shown by balls with other different colors.

S2. PDOSs of α, and β tellurene phases decorated adatoms

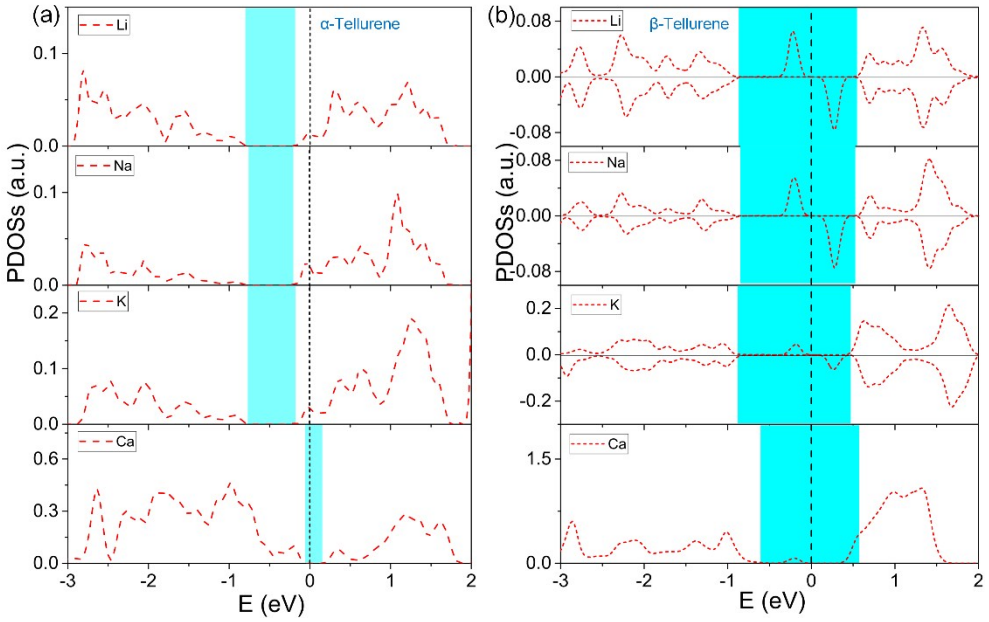

Figure. S2 PDOSs of α, and β tellurene phases decorated with alkali and alkali-earth adatoms (Li, Na, K, and Ca). The vertical dotted lines denote the Fermi level and the light blue rectangles denote the band gap.

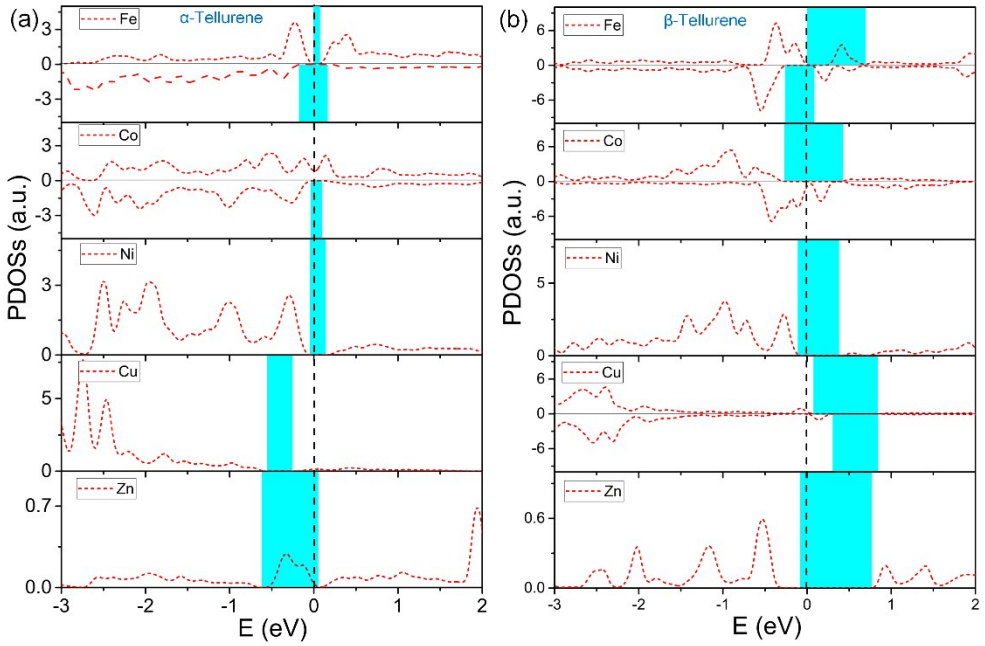

Figure. S2 DOSs of α, and β tellurene phases decorated with transition metal adatoms (Fe, Co, Ni, Cu, and Zn). The vertical dotted lines denote the Fermi level and the light blue rectangles denote the band gap.

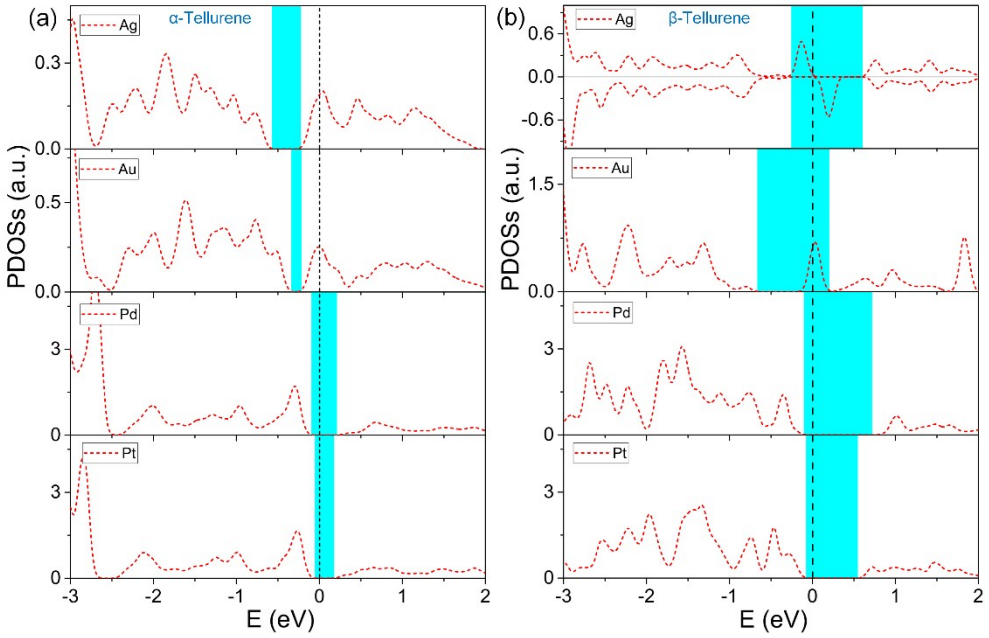

Figure. S2 PDOSs of α, and β tellurene phases decorated with noble metal adatoms (Ag, Au, Pd, and Pt). The vertical dotted lines denote the Fermi level and the light blue rectangles denote the band gap.

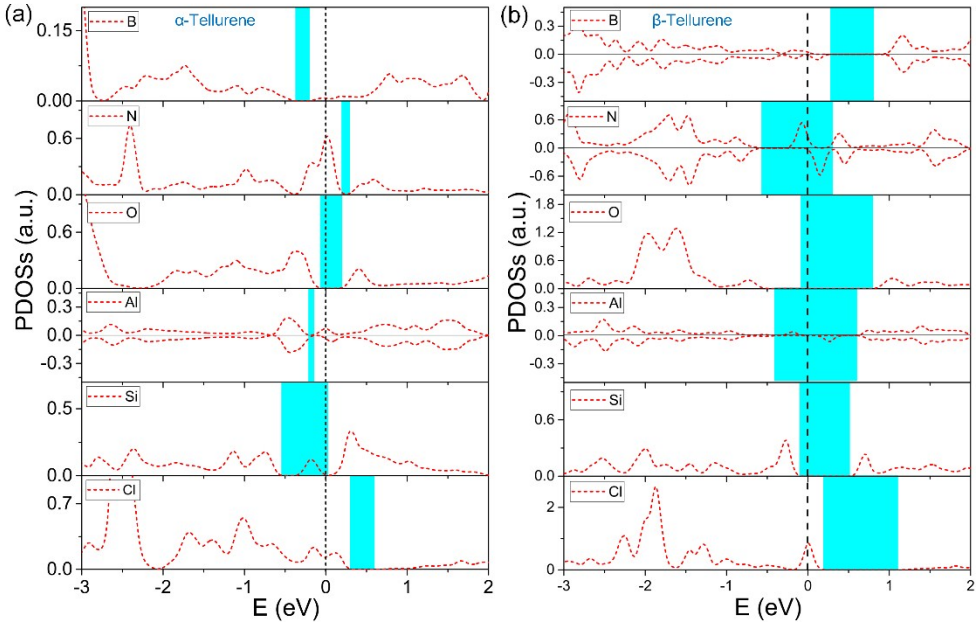

Figure. S2 PDOSs of α, and β tellurene phases decorated with nometallic adatoms (B, N, O, Si, Cl) and Al adatom. The vertical dotted lines denote the Fermi level and the light blue rectangles denote the band gap.

S3. Cohesive energy and adsorption energy of metal adatoms

Element	Cohesive energy (DFT work)	Cohesive energy (exp[1])	Adsorption energy (α--Te)	Adsorption energy (α--Te)	Agglomeration (α-Te)	Agglomeration (β-Te)
Li	1.55	1.63	-2.238	-2.346	no	no
Na	1.06	1.113	-1.755	-1.823	no	no
K	0.84	0.934	-1.922	-2.031	no	no
Ca	1.73	1.84	-3.901	-2.86	no	no
Fe	4.93	4.28	-4.618	-3.842	yes	yes
Co	5.06	4.39	-4.931	-2.828	yes	yes
Ni	4.83	4.44	-3.1	-4.67	yes	yes
Cu	3.27	3.49	-2.757	-2.74	yes	yes
Zn	1.23	1.35	-0.569	-0.364	yes	yes
Ag	2.54	2.95	-1.976	-1.334	yes	yes
Au	3.02	3.81	-2.534	-1.68	yes	yes
Pd	3.72	3.89	-3.878	-3.289	no	yes
Pt	5.44	5.84	-5.544	-4.199	no	yes
Al	3.26	3.39	-2.754	-3.42	yes	no

References:

1. C. Kittel, Introduction to Solid State Physics, 8th edn., Wiley, 2004.