Ohmic-to-Schottky Conversion in Monolayer Tellurene–Metal Interface via Graphene Insertion

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Table S1. Parameters for interfaces formed using ML tellurene, graphene and metal surfaces. The first column gives the angle of rotation between two surfaces while aligning and second column specifies the mean strain applied on the surfaces during matching. Third and fourth column show the surface area and angle between the vectors of created interface supercells. For generating tellurene–graphene–metal interfaces, strain is applied only on the metal surfaces. To build tellurene–graphene–metal heterostructures, interfaces between metal and graphene surfaces are initially formed in which both the surfaces are strained. These combined graphene–metal surfaces are then interfaced with tellurene where strain is applied on graphene–metal surface only.

Interface	Rotation angle between two surfaces (degree)	Mean strain (%)	Surface Area of interface supercell (nm^2)	Angle between two vectors of interface supercell (degree)
Au-Te	56.39	0.80	1.89	67.23
Ag-Te	4.70	0.61	1.89	112.81
Pd-Te	75.03	0.45	2.60	114.18
Pt-Te	120.06	0.54	1.42	76.17

Ru-Te	25.99	0.70	1.18	71.26
Ti-Te	56.94	0.62	2.37	57.45
C-Te	90.76	0.61	1.89	60.76
Au-C	90	0.97	0.21	120
AuC-Te	89.79	0.30	1.90	60.57
Ag-C	150	0.47	0.21	120
AgC-Te	149.65	0.80	1.89	119.65
Pd-C	160.89	0.56	0.47	60.42
PdC-Te	29.43	0.50	2.85	60.57
Pt-C	150	0.80	0.21	120
PtC-Te	29.79	0.49	1.42	126.80
Ru-C	150	1.64	0.21	61.20
RuC-Te	30	0.54	1.42	104.07
Ti-C	166.10	0.33	0.68	120
TiC-Te	138.28	1.97	2.60	120.18

Table S2. Comparisons of workfunctions of combined tellurene–metal systems calculated using VASP and QuantumATK.

Structure	VASP calculated WF (eV)	QuantumATK calculated WF (eV)
AuTe	4.83	5.12
AgTe	4.58	4.20
PdTe	4.97	5.35
PtTe	5.76	5.61
RuTe	5.12	5.08
TiTe	4.59	4.54

Table S3. Bader charge analysis in tellurene–graphene–metal composite systems. Q_{Te} and Q_{MCTe} represent Bader charges calculated using VASP in pristine tellurene and tellurene layer in the composite systems, respectively. Δ_Q denotes loss of charge in tellurene when interfaced with graphene-metal surfaces ($\Delta_Q = Q_{MCTe} - Q_{Te}$).

Interface	Q_{Te} (e)	Q_{MCTe} (e)	Δ_Q (e)
Au-C-Te	144	143.936	-0.064
Ag-C-Te	144	143.928	-0.072
Pd-C-Te	216	215.829	-0.171
Pt-C-Te	108	107.882	-0.118
Ru-C-Te	108	107.937	-0.063
Ti-C-Te	198	197.883	-0.117

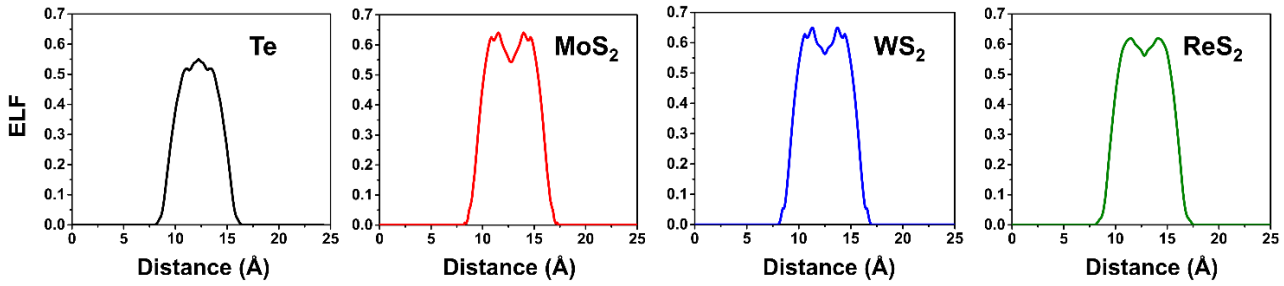

Figure S1. Comparisons of electron localization functions between monolayer Te, MoS_2, WS_2 and ReS_2. For tellurene the value is lower compared to 2D transition metal di chalcogenides implying more delocalized electrons, hence more chemical reactivity.

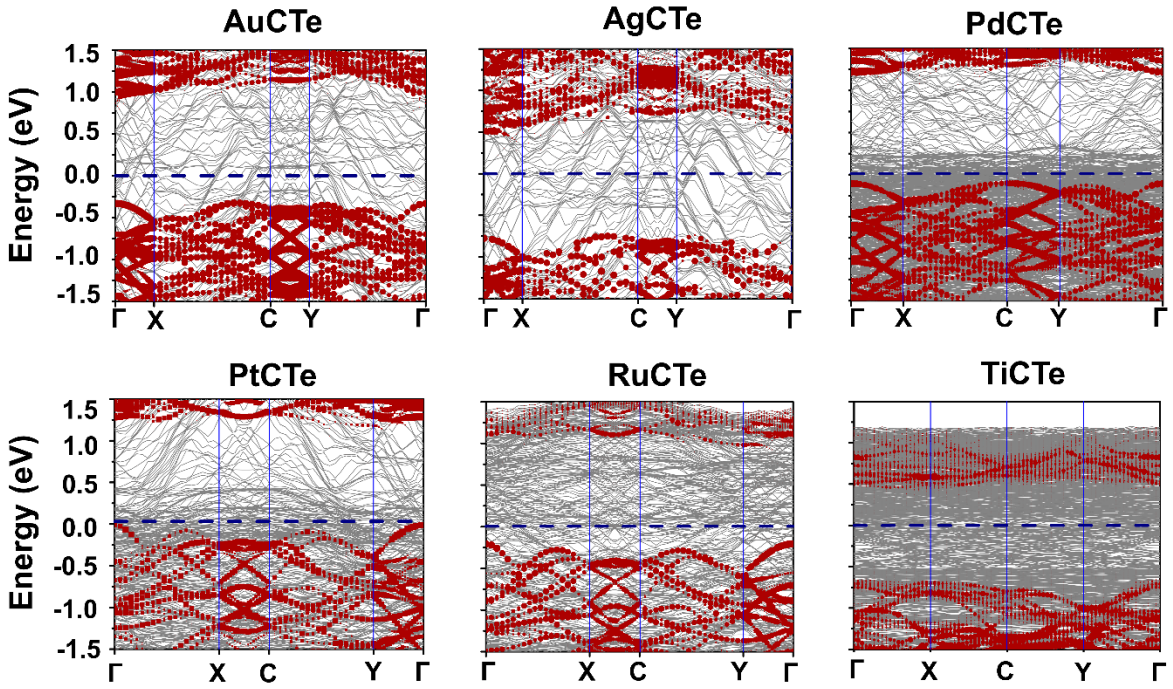

Figure S2. Band structures of ML tellurene–graphene–metal calculated using VASP plane wave DFT package. Red lines denote the bands projected to tellurene. Fermi level is set at zero energy and represented by blue dashed line. For Au, Pd, Pt and Ti the valence bands of tellurene come close to Fermi level (p-type) but for Ag and Ti conduction bands to the Fermi level (n type). For Ag and Ti the projected band structures contradict the Bader charge results. According to Bader charge analysis, for all metals tellurene make p-type contact with graphene-metal surfaces.