Table 2 Comparison of Ionization potentials (IP) and Electron affinities (EA) of 17 semiconducting and insulating materials from this work and the values from Photoemission, estimated IPs and EAs using Mulliken electronegativity scale (see eq.(3) and Ref.[9]), and values from electrochemical measurements (at pH=1). Results from this work are surface orientation dependent and therefore, we specify the (hkl) surface orientation and provide the corresponding surface energies E_{hkl}.

		This work					Photoemission[a]		From Mulliken electronegativities		Electrochemistry[b] pH=1	
	(hkl)	E_g [eV]	IP [eV]	EA [eV]	E_{hkl} [eV/Å^2]	E_g^a [eV]	IP [eV]	EA [eV]	IP [eV]	EA [eV]	IP [eV]	EA [eV]
GaN	$(10\bar{1}0)$		6.78	3.52	0.096							
GaN	$(11\bar{2}0)$	3.26	6.73	3.47	0.102	3.4	6.0 – 6.9[c]	2.6 – 3.5[c]	6.49	3.09	6.67[d] – 7.50[d]	3.53[d] – 4.10[d]
GaAs	(110)	1.20	5.49	4.30	0.026	1.42	5.56	4.14	4.80	3.38	4.96 – 5.51	3.61 – 4.08
GaP	(110)	2.56	6.37	3.82	0.041	2.27	6.01	3.74	5.34	3.07	5.60 – 5.83	3.38 – 3.60
InP	(110)	1.28	6.09	4.81	0.032	1.34	5.85	4.51	4.80	3.46	5.63	4.29
SnO_2	(110)	3.43	9.13	5.70	0.064	3.6	8.9[e]	5.3	8.01	4.41	8.10 – 8.55	4.63 – 4.91
SnO_2	(100)		9.16	5.73	0.069							
SnO_2	(101)		8.66	5.23	0.089							
SnO_2	(001)		7.47	4.04	0.114							
ZnO	$(10\bar{1}0)$		7.53	4.30	0.054							
ZnO	$(11\bar{2}0)$	3.23	7.60	4.37	0.056	3.4	7.82	4.42	7.65	4.25	7.38 – 7.77[l]	4.23 – 4.37[l]
ZnS	(110)	3.69	7.57	3.88	0.026	3.7	7.5	3.8	7.25	3.55		
ZnSe	(110)	2.61	6.77	4.16	0.018	2.7	6.82	4.12	6.61	4.16	5.74	3.04
CdS	$(10\bar{1}0)$		7.20	4.75	0.020							
CdS	$(11\bar{2}0)$	2.45	7.15	4.70	0.020	2.6	7.26	4.66	6.58	3.98	5.14 – 6.50	2.70 – 4.12
CdSe	$(10\bar{1}0)$		6.42	4.74	0.011							
CdSe	$(11\bar{2}0)$	1.68	6.38	4.70	0.011	1.75	6.62	4.87	6.02	4.27	6.02 – 6.18	4.21 – 4.41
$TiO_2^{rut.}$	(110)	2.84	7.51	4.67	0.044	3.03			7.32	4.30	7.25 – 7.47	4.28 – 4.44
$TiO_2^{rut.}$	(100)		7.78	4.94	0.055							
$TiO_2^{rut.}$	(101)		6.93	4.09	0.074							
$TiO_2^{rut.}$	(001)		5.58	2.74	0.095							
$TiO_2^{ana.}$	(101)	3.20	7.82	4.62	0.041	3.23			7.42	4.19	7.25 – 7.47	4.28 – 4.42
MnO	(100)	3.27	5.08	1.80	0.040	3.5[f]			7.04	3.54		
NiO	(100)	3.41	4.98	1.80	0.053	3.5[f]			7.51	4.01	5.33[g]	1.73[g]
Cu_2O	(111)	2.03	5.49	3.46	0.046	2.2[f]	5.66[h]	3.56[h]	6.42	4.22	5.61[i]	3.41[i]
Fe_2O_3	$(01\bar{1}2)$	1.81	6.70	4.89	0.064	2.1[f]			6.92	4.82	6.95	4.85
Fe_2O_3	(0001)		5.70	3.89	0.069							
$SrTiO_3$	(001)*	3.14	6.71	3.57	0.065	3.2	7.1[j] – 7.5[k]	3.9[j] – 4.3[k]	6.92	3.72	7.28[l] – 7.64	4.08[l] – 4.44
$SrTiO_3$	(001)**		4.41	1.27	0.065							

*TiO_2 terminted, **SrO terminated

[a]Ref.[33] if not stated otherwise; [b]Refs.[5,6,8,20,57] if not stated otherwise

[c]Ref.[36] and the references therein; [d]Ref.[58]; [e]Ref.[69]; [f]Ref.[26] and the references therein; [g]Ref.[60]; [h]Ref.[37]; [i]Ref.[61]; [j]Ref.[38]; [k]Ref.[39,40]

[l]Ref.[59]

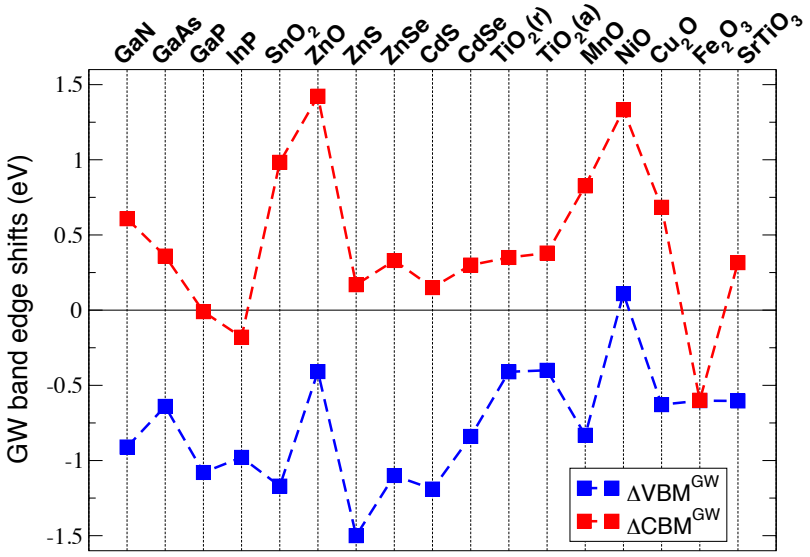

Fig. 7 Calculated GW band edge shifts ΔVBM and ΔCBM relative to the base GGA+U calculations for 17 materials studied in this work.