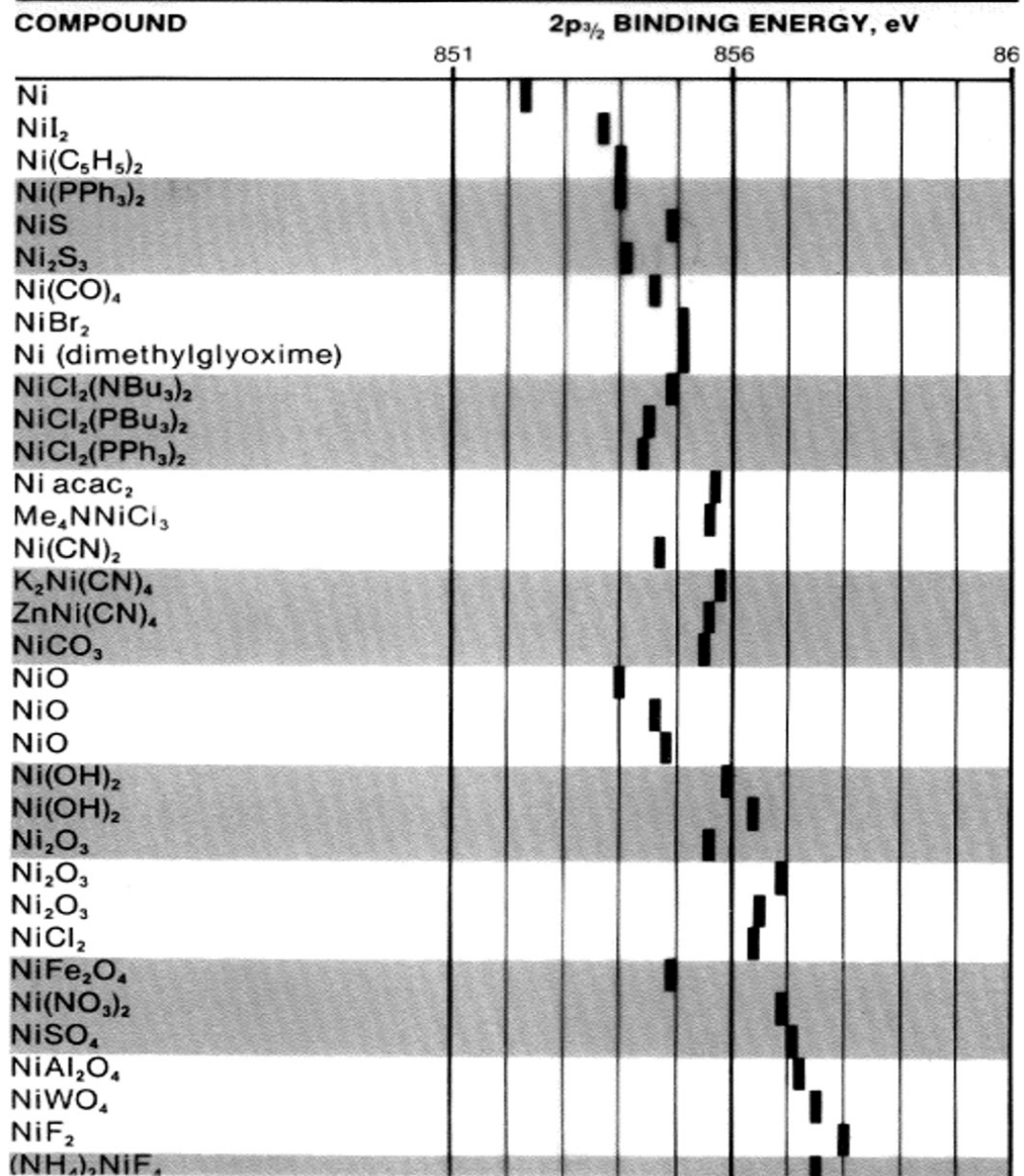
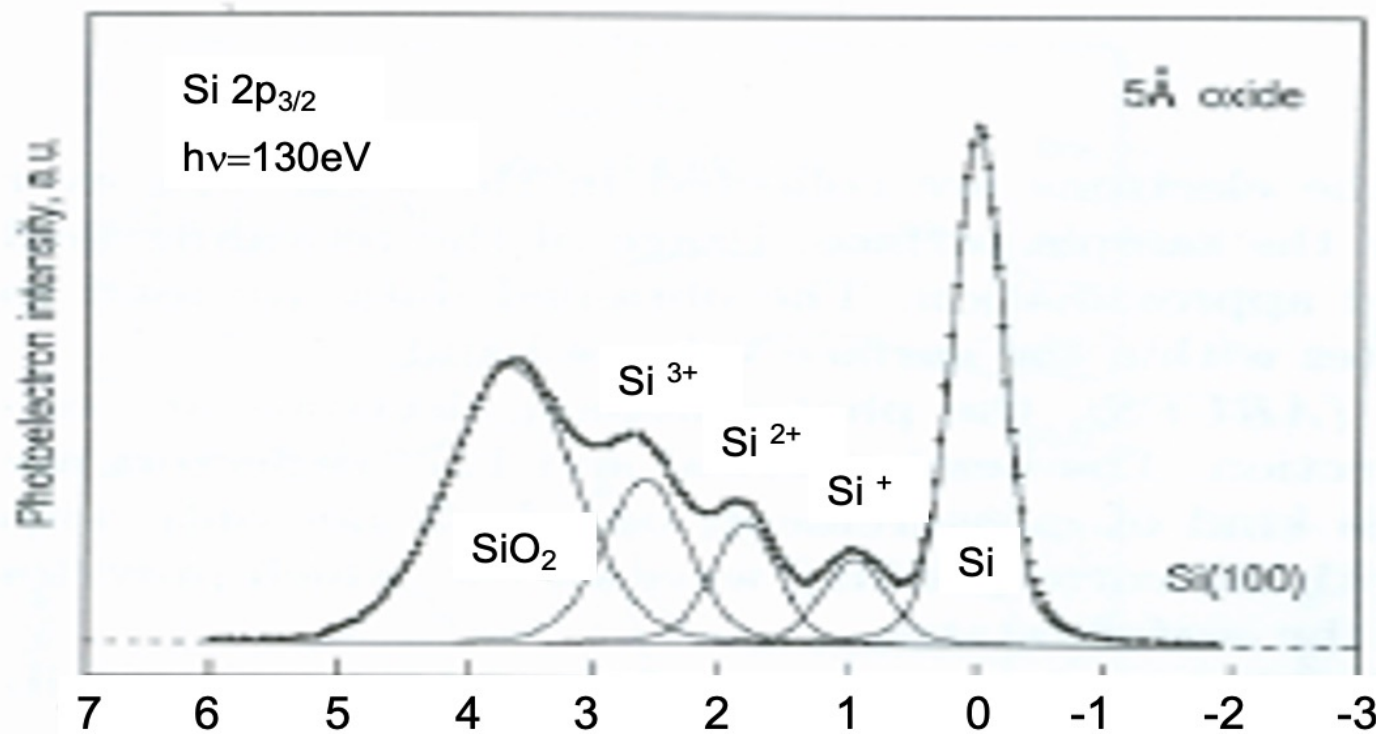


Nickel, Ni

Atomic Number 28





UPS Relative BE of Si: 5Å oxide on Si (100)
higher BE with increasing oxidation state.

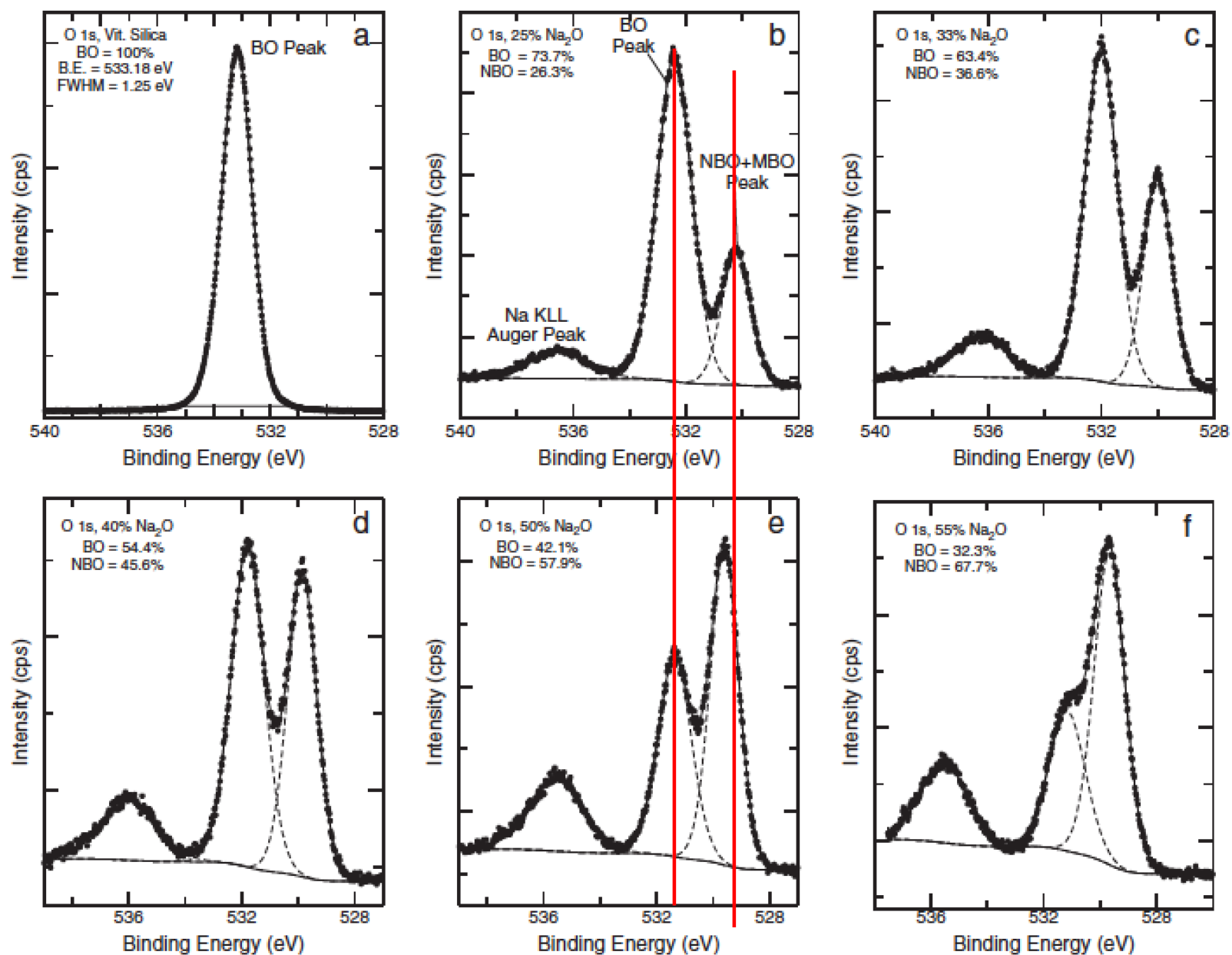


Table 1. Calculated charges (Q), percent mixing, and E_{A-B} values for the molecule $RH_5Si_2O_7$ ¹ and ΔG for reaction (1)

R atom	K ²	Na	Li	H
Q(R)	0.894	0.753	0.490	0.153
Q(O(br))	-0.723	-0.729	-0.737	-0.744
Q(O(nbr)) ₃	-0.720	-0.713	-0.671	-0.614
Q(Si)	1.348	1.441	1.563	1.730
% mixing R ⁴ ₅	1.3	3.1	6.4	42.3
E_{R-O}	-1.295	-5.111	-14.027	-21.678
$E_{Si-O(br)}$	-12.072	-13.137	-14.747	-17.121
$E_{Si-O(nbr)}$ ₆	-17.763	-17.233	-17.251	-15.024
ΔG	+463	+431	+307	0

Table 3a. Calculated charges(Q), % mixing, E_{A-B} values (eV) for the molecule $(RH_6Si_2O_7)^{1+}$ ¹, and ΔG for reaction (3a)

R atom	K	Na	Li	H
Q(R)	0.936	0.741	0.571	0.218
Q(O(br))	-0.780	-0.767	-0.734	-0.561
Q(Si)	1.728	1.737	1.767	1.773
% mixing R	0.8	3.2	5.4	39.1
$E_{R-O(br)}$	0.089	-2.780	-9.139	-20.629
$E_{Si-O(br)}$	-17.158	-16.225	-14.982	-9.308
ΔG ²	-0.5	-23	-111	-317