Electronic Supplementary Information

Palladium decorated SiX (X = N, P, As, Sb, Bi) Catalysts for Hydrogen Evolution

Trilokchand L. Kumavat[a], Radha N Somaiya[b,*], Yogesh Sonvane[a,*]

[a]*Advanced Materials Lab, Department of Physics, Sardar Vallabhbhai National Institute of Technology, Surat 395007, India*
[b]*Department of Physics, Indian Institute of Technology Bombay, Powai, Mumbai 400076, India*

*Corresponding Author(s): somaiyaradha@gmail.com; yas@phy.svnit.ac.in

Figure Captions:

Fig. S1: Electronic band Structure calculated using PBE (red dotted lines) and HSE06 (blue solid lines) functional and PDOS of (a, b) SiN, (c, d) SiP, (e, f) SiAs, (g, h) SiSb and (i, j) SiBi binary compounds, respectively. The Fermi level is set to zero.

Fig. S2: Electronic band structure calculated using PBE functional and PDOS of (a-c) Pd@SiN, (d-f) Pd@SiP, (g-i) Pd@SiAs, (j-l) Pd@SiSb and (m-o) Pd@SiBi SACs, respectively. The Fermi level is set to zero. The inset indicates that the valence band of Pd@SiN SAC is not flat.

Fig. S3: Electronic Band Structure after H-adsorption of (a) Pd@SiN, (b) Pd@SiP, (c) Pd@SiAs, (d) Pd@SiSb and (e) Pd@SiBi SACs, respectively. The Fermi level is set to zero. The inset indicates that the valence band of Pd@SiN SAC is not flat.

Fig. S4: Projected DOS after H-adsorption of (a-c) Pd@SiN, (d-f) Pd@SiP, (g-i) Pd@SiAs, (j-l) Pd@SiSb and (m-o) Pd@SiBi SACs, respectively. The Fermi level is set to zero.

Table Captions:

Table S1: Optimized structural properties (bond lengths and bond angles) of pristine SiX (X = Group-V) binary compounds, Pd@SiX SACs and H adsorbed Pd@SiX SACs.

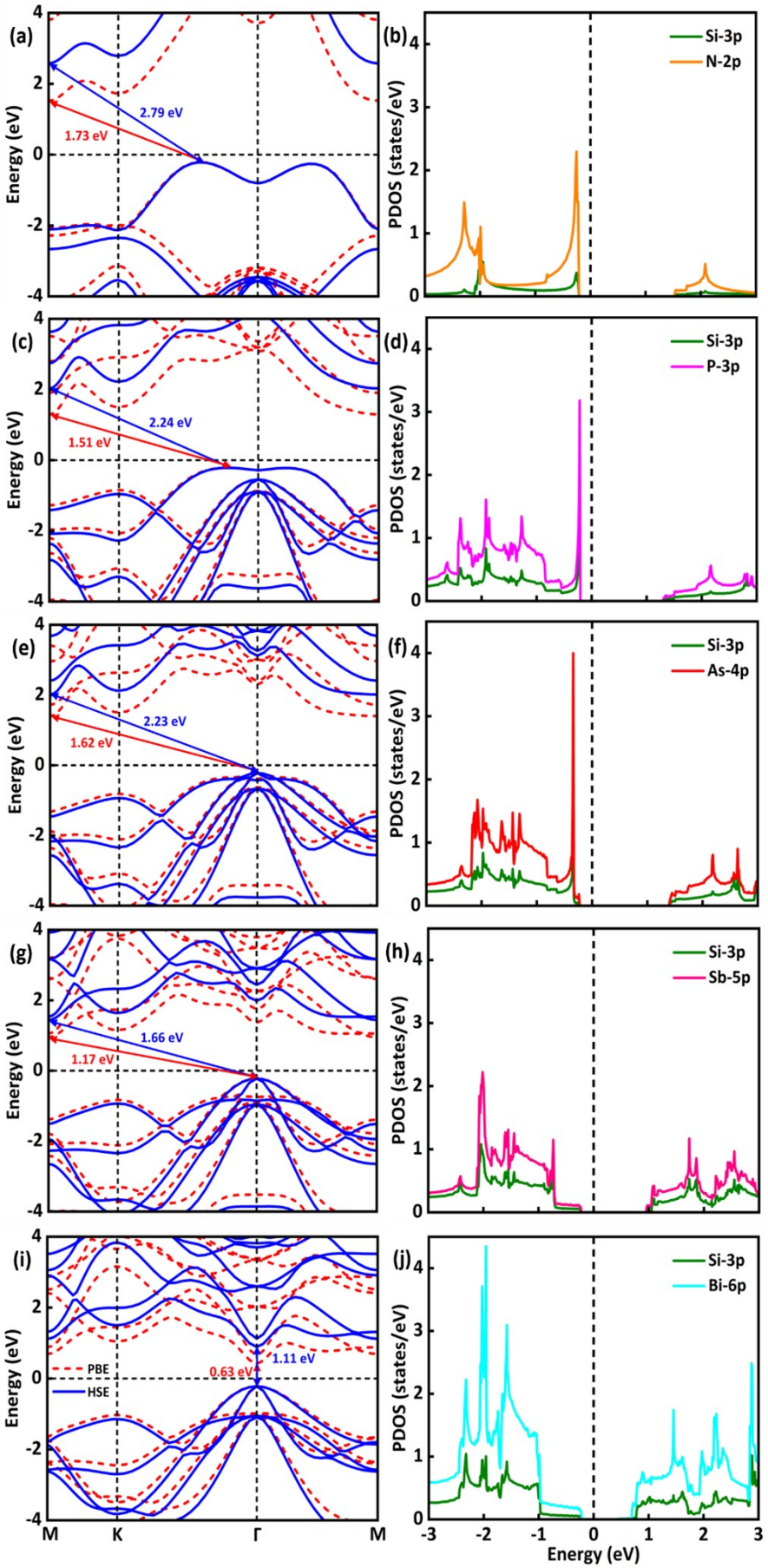
(a)
(b)
(c)
(d)
(e)
(f)
(g)
(h)
(i)
(j)
Energy (eV)
PDOS (states/eV)
2.79 eV
1.73 eV
2.24 eV
1.51 eV
2.23 eV
1.62 eV
1.66 eV
1.17 eV
1.11 eV
0.63 eV
PBE
HSE
Si-3p
N-2p
P-3p
As-4p
Sb-5p
Bi-6p
M
K
Γ
M
Energy (eV)

Fig. S1

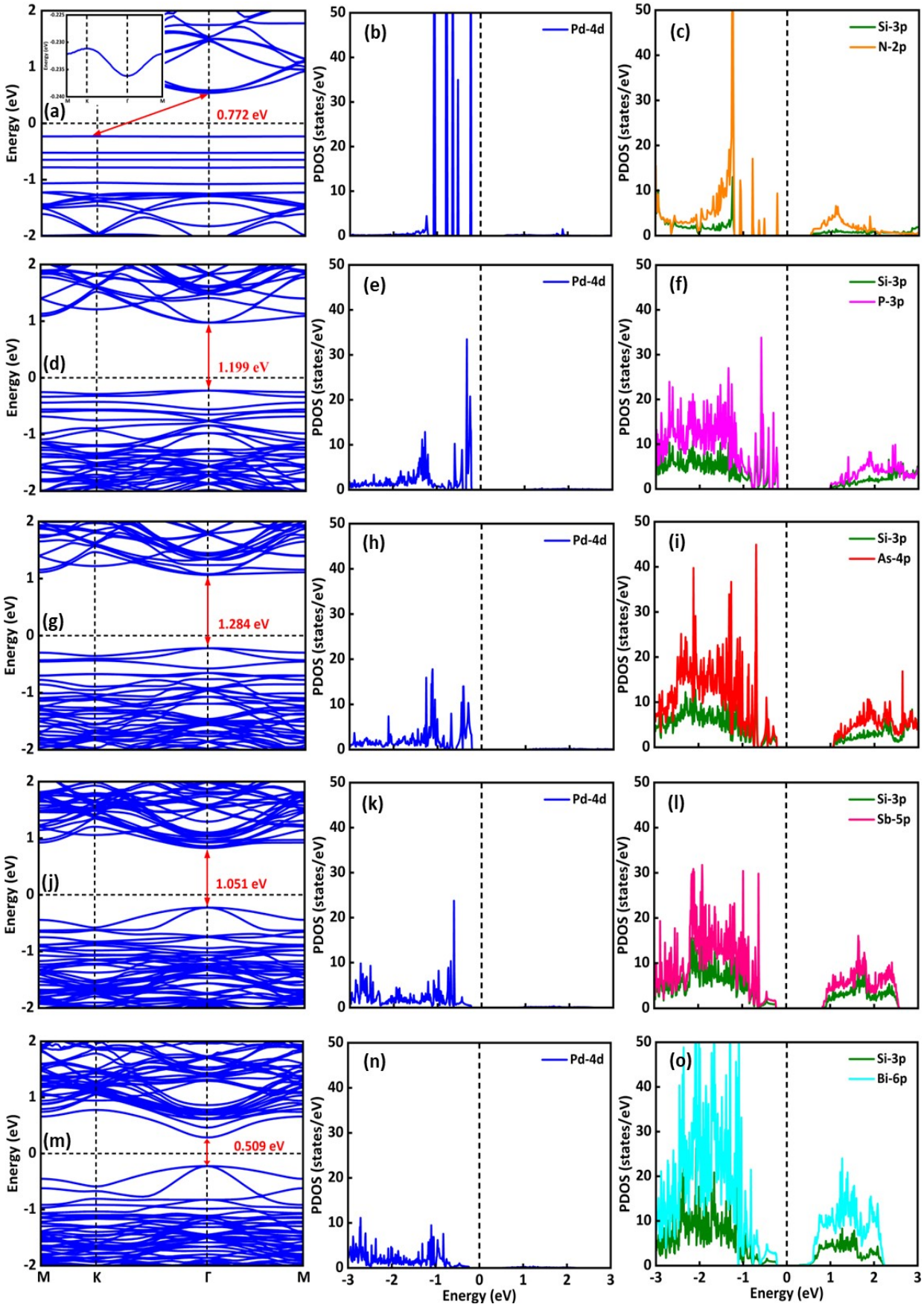
(a)
0.772 eV
(b)
Pd-4d
(c)
Si-3p
N-2p
(d)
1.199 eV
(e)
Pd-4d
(f)
Si-3p
P-3p
(g)
1.284 eV
(h)
Pd-4d
(i)
Si-3p
As-4p
(j)
1.051 eV
(k)
Pd-4d
(l)
Si-3p
Sb-5p
(m)
0.509 eV
(n)
Pd-4d
(o)
Si-3p
Bi-6p
Energy (eV)
PDOS (states/eV)
M
K
Γ
M

Fig. S2

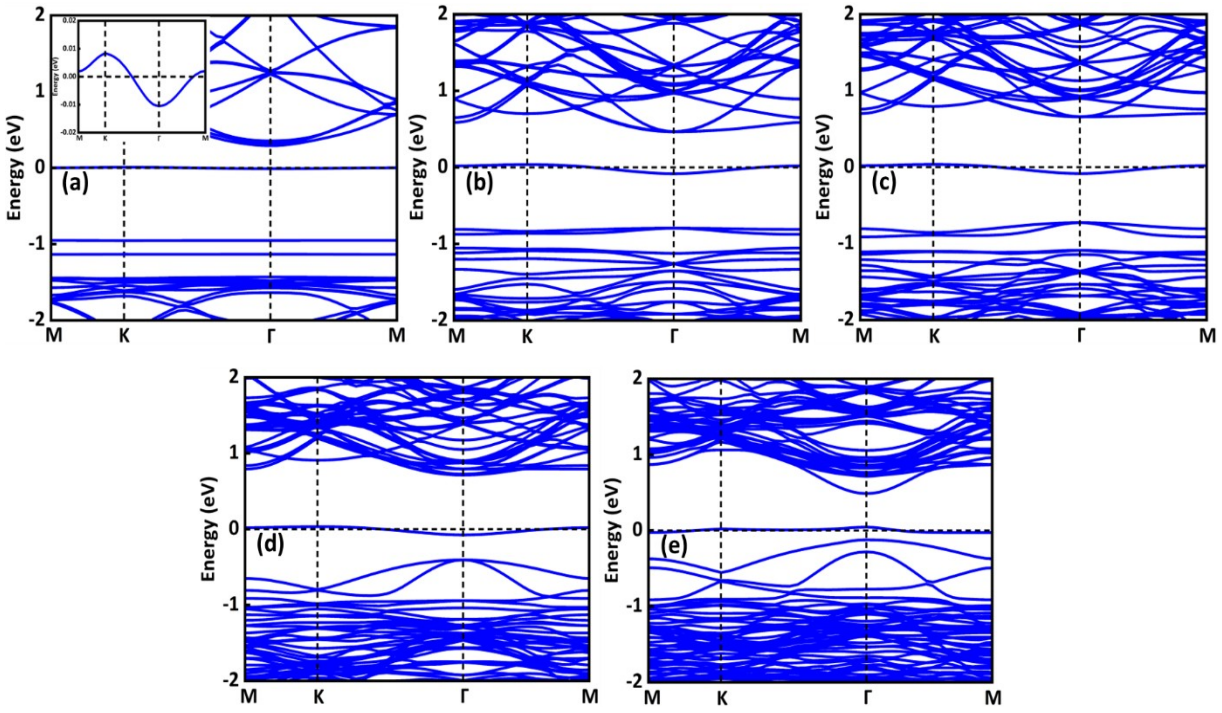

Fig. S3

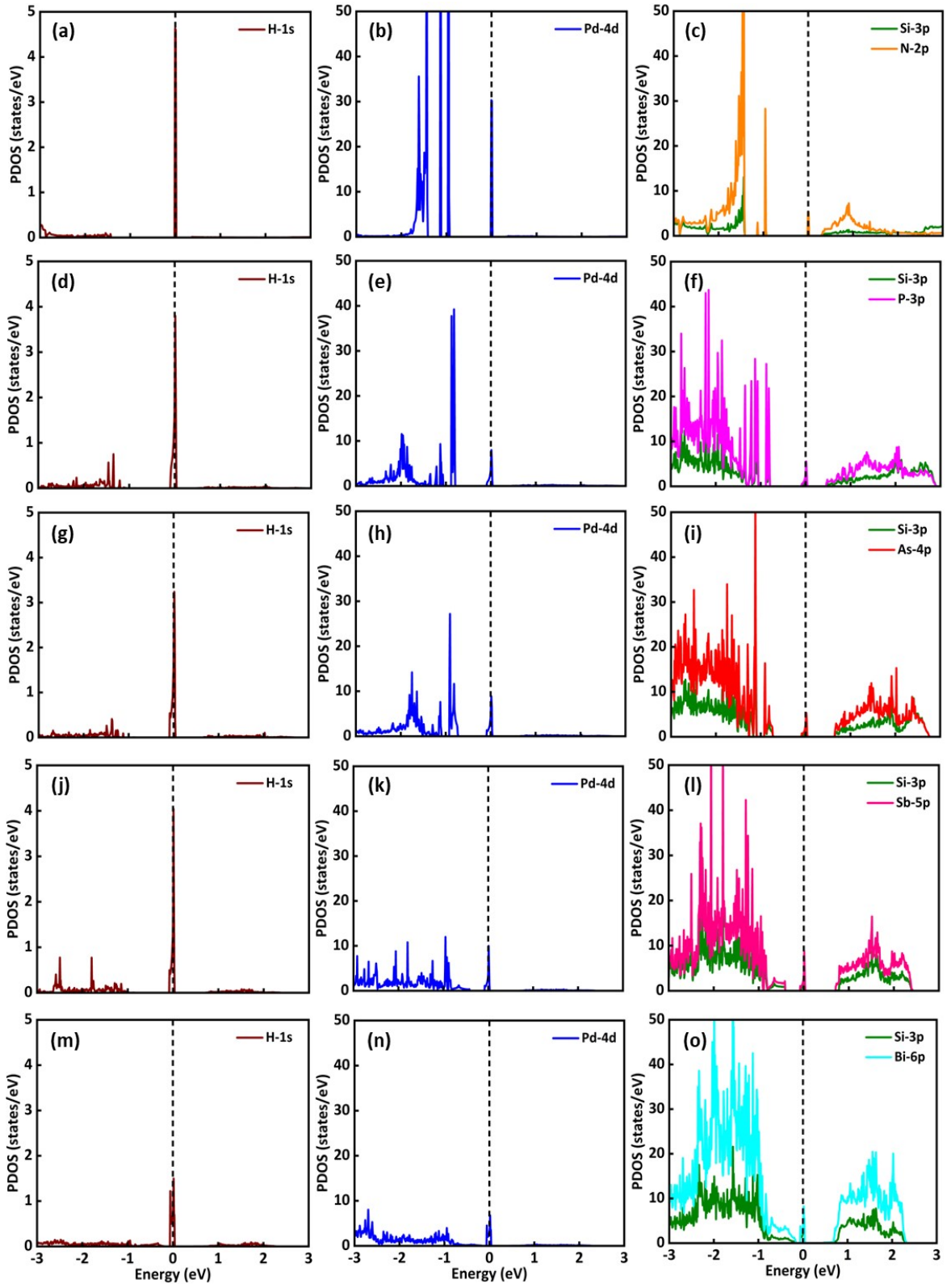
(a)
H-1s
(b)
Pd-4d
(c)
Si-3p
N-2p
(d)
H-1s
(e)
Pd-4d
(f)
Si-3p
P-3p
(g)
H-1s
(h)
Pd-4d
(i)
Si-3p
As-4p
(j)
H-1s
(k)
Pd-4d
(l)
Si-3p
Sb-5p
(m)
H-1s
(n)
Pd-4d
(o)
Si-3p
Bi-6p
PDOS (states/eV)
Energy (eV)

Fig. S4

Table S1

System	Bond length (Å)			Bond angle (°)	
	Si-Si	X-X	Si-X	θ_1 (Si-Si-X)	θ_2 (Si-X-Si)
SiN	2.42	3.53	1.76	108.34	110.57
Pd@SiN	2.44	3.52	1.77	106.45	110.91
H-Pd@SiN	2.43	3.53	1.76	108.20	110.73
SiP	2.37	4.39	2.27	116.40	101.73
Pd@SiP	2.35	4.38	2.28	117.60	101.79
H-Pd@SiP	2.36	4.38	2.28	116.83	101.78
SiAs	2.35	4.56	2.39	117.35	100.55
Pd@SiAs	2.34	4.55	2.40	117.12	101.02
H-Pd@SiAs	2.35	4.55	2.40	117.27	100.76
SiSb	2.35	4.80	2.61	117.89	99.88
Pd@SiSb	2.34	4.79	2.64	116.94	100.28
H-Pd@SiSb	2.34	4.79	2.63	117.69	100.27
SiBi	2.34	4.89	2.72	117.89	99.88
Pd@SiBi	2.33	4.88	2.77	116.71	99.99
H-Pd@SiBi	2.33	4.90	2.76	118.46	99.81