

Supporting Information

Hydrophobic and antioxydant effects in In, Sn, and Sb based two dimensional materials

Keisuke Takahashi*

*Graduate School of Engineering, Hokkaido University,
N-13, W-8, Sapporo 060-8628, Japan*

Lauren Takahashi

Freelance Researcher, Central Ward, Sapporo 064, Japan

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* keisuke.takahashi@eng.hokudai.ac.jp

Table I shows the adsorption energies of O₂ and H₂O over Sn, SnSb, InSb, InSn, and bulk Sn(100), In(100), and Sb(100). Figure 1 shows the atomic models of relaxed H₂O and O₂ adsorption sites over two dimensional Sn, SnSb, InSb, and InSn.

	O ₂	H ₂ O
Sn	-2.17 (-50.04)	-0.81(-18.68)
InSb(In)	-1.24(-28.60)	-0.72(-16.60)
InSb(Sb)	-0.36(-8.30)	-0.40(-9.22)
SnSb(Sn)	-1.70(-39.20)	-0.69(-15.91)
SnSb(Sb)	-1.40(-32.29)	-0.06(-1.38)
InSn(Sn)	-8.48(-195.55)	-5.24(-120.84)
InSn(In)	-9.73(-224.38)	-5.11(-117.84)
Sn(100)	-5.28(-121.76)	-3.89(-89.706)
In(100)	-7.45(-173.88)	-3.43(-79.10)
Sb(100)	-2.02(-46.58)	-0.51(-11.76)

TABLE I: Adsorption energies in eV (kcal/mol) of O₂ and H₂O over Sn, SnSb, InSb, InSn, and bulk Sn(100), In(100), and Sb(100).

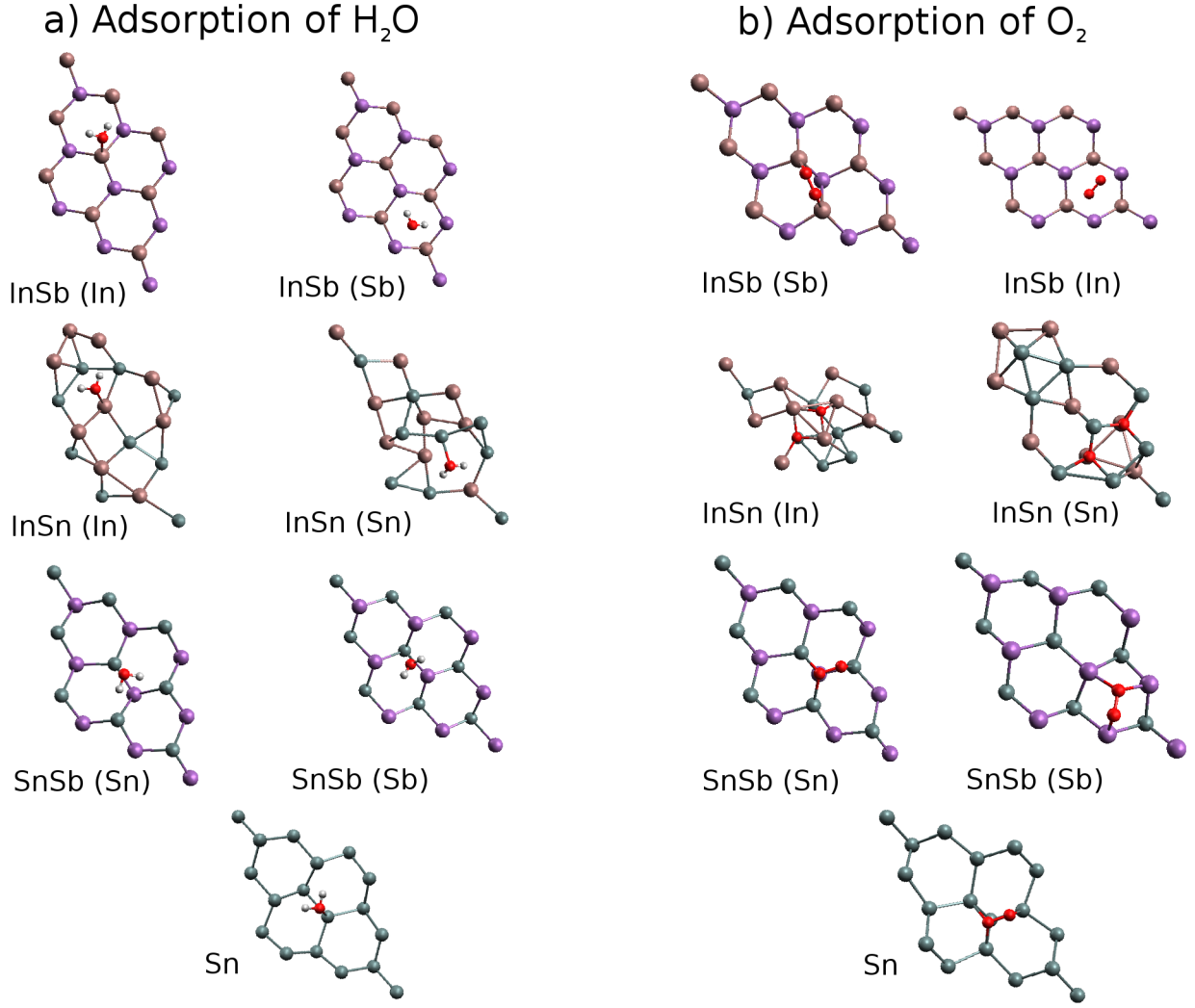


FIG. 1: Atomic models of relaxed (a) H_2O and (b) O_2 adsorption sites over two dimensional Sn, SnSb, InSb, and InSn. Atom colors are as follows: Gray-Sn, In-Brown, Sb-Purple, Red-O, White-H.