Electronic Supplementary Material (ESI) for Nanoscale.

Supplementary materials on:

Searching for Large-gap Quantum Spin Hall Insulators in Sandwiched Boron-Nitride/(Pb, Sn)/α-Al_2O_3 Structures

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TABLE S1. The binding energy (E_b) of BN, distance between Al and atop-Pb ($d_{Al\text{-}Pb}$), BN and atop Pb ($d_{BN\text{-}Pb}$), and bond length ($d_{Pb\text{-}Pb}$) at different adsorption sites, respectively.

BN	E_b (eV)	$d_{Al\text{-}Pb}$ (Å)	$d_{BN\text{-}Pb}$ (Å)	$d_{Pb\text{-}Pb}$ (Å)
T	-0.28	3.07	3.61	3.05
H	-0.29	3.07	3.53	3.05
B	-0.28	3.07	3.57	3.05

TABLE S2. The binding energy (E_b) of BN, distance between Al and atop-Sn ($d_{Al\text{-}Sn}$), BN and atop-Sn ($d_{BN\text{-}Sn}$), and bond length ($d_{Sn\text{-}Sn}$) at different adsorption sites, respectively.

BN	E_b (eV)	$d_{Al\text{-}Sn}$ (Å)	$d_{BN\text{-}Sn}$ (Å)	$d_{Sn\text{-}Sn}$ (Å)
T	-0.24	2.87	3.64	3.03
H	-0.25	2.88	3.55	3.03
B	-0.24	2.88	3.58	3.03

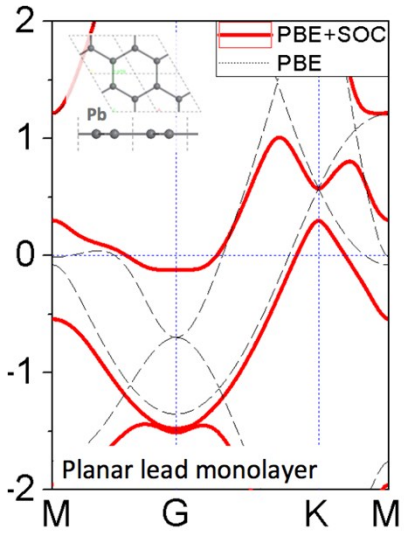

Fig S1 (color online) Electronic band structures planar lead monolayer with (red thick line) and without (back thin line) SOC. Insets demonstrate the top and side view of atomic structures with a lattice constant of 5.159 Å. Horizontal blue-dashed line indicates the Fermi level.

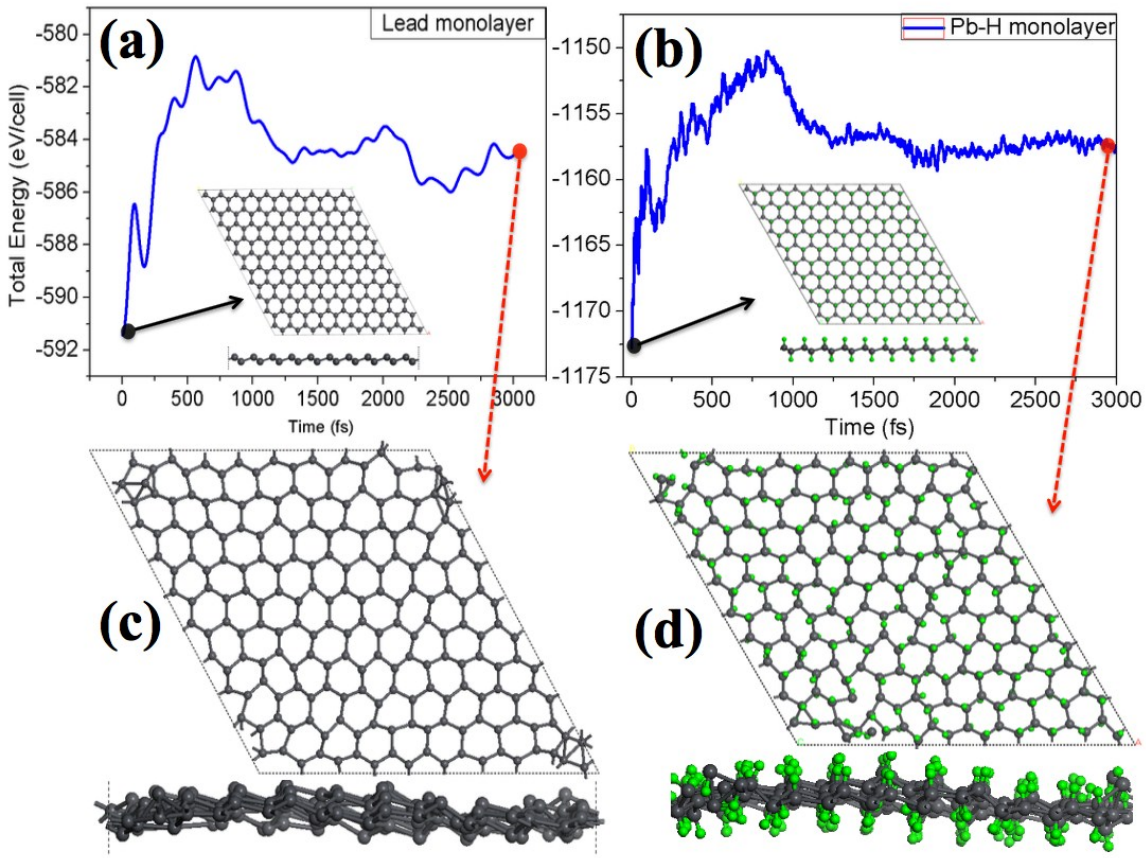

Fig S2 (color onine) Ab initio molecular dynamic simulation of monolayer (a) "Pb" and (b) "Pb-H" with a period of 3 pico seconds. Insets demonstrate the initial atomic structures. (c) and (d) represent snapshots of corresponding to the final structures obtained from AIMD.

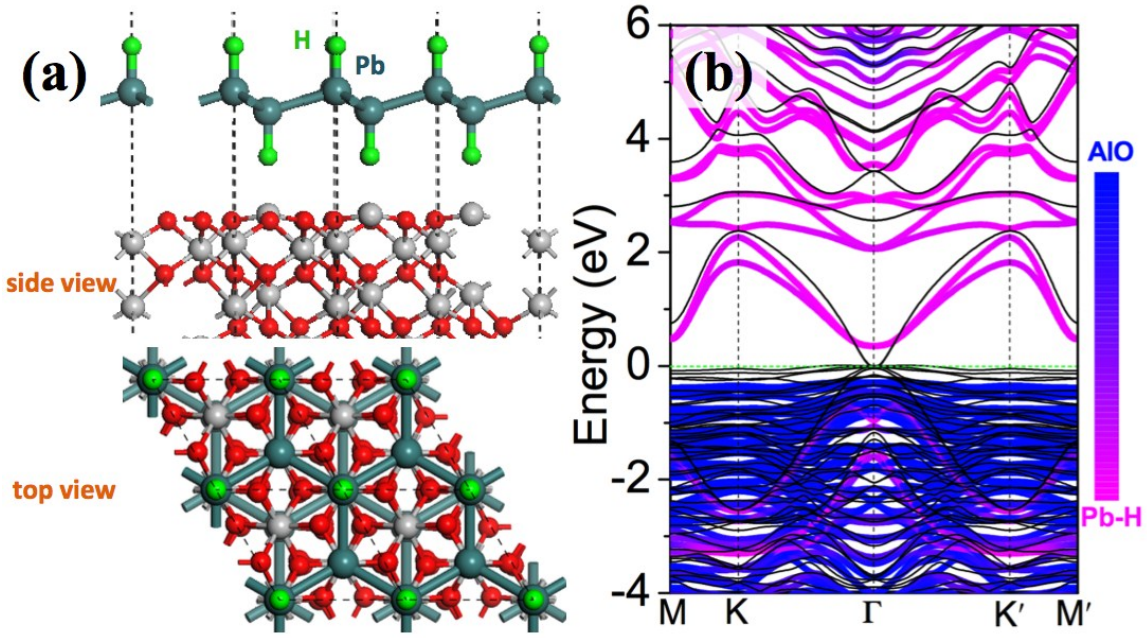

Fig S3 (color onine) (a) Side and top view for the atomic structures of Pb-H/Al_2O_3. (b) Electronic band structures of Pb-H monolayer adsorbed on α-alumina surface with (color thick line) and without (back thin line) SOC. The color bar indicates the contributions from Pb-H layers (pink) and α-alumina substrate (blue), with the atomic contributions computed by projecting the Bloch wave functions of Pb-H/Al_2O_3 into Pb-H atoms. Horizontal green-dashed line indicates the Fermi level.

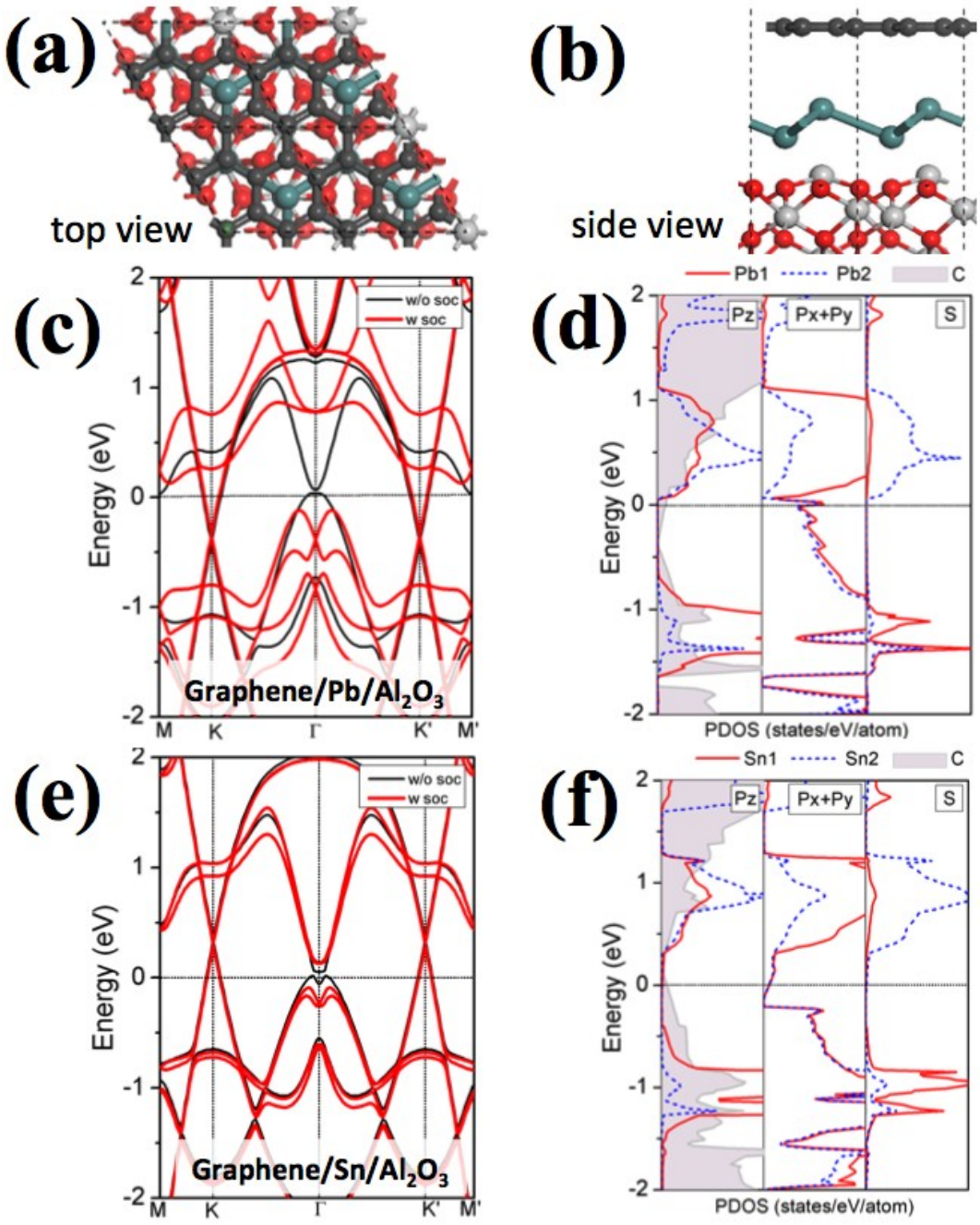

Fig. S4 (color online) (a) Top and (b) side view of sandwiched graphene/(Pb, Sn)Al_2O_3 structures. Electronic band structures of (c) graphene/Pb/ Al_2O_3 and (e) graphene/Sn/Al_2O_3 sandwiched structures with (thick red solid lines) and without (thin black line) spin orbit coupling in calculations. (d) and (f) are the corresponding atomic-orbital projected local density of states of C, Pb and Sn atoms, where C, Pb and Sn atoms are demonstrated for the p_z, p_x+p_y and s orbitals, respectively.