Supplementary Information (SI) for Journal of Materials Chemistry C.

Quantum spin Hall effect and tunable topological states in M_2O_3 (M = Nb, Ta) bilayers

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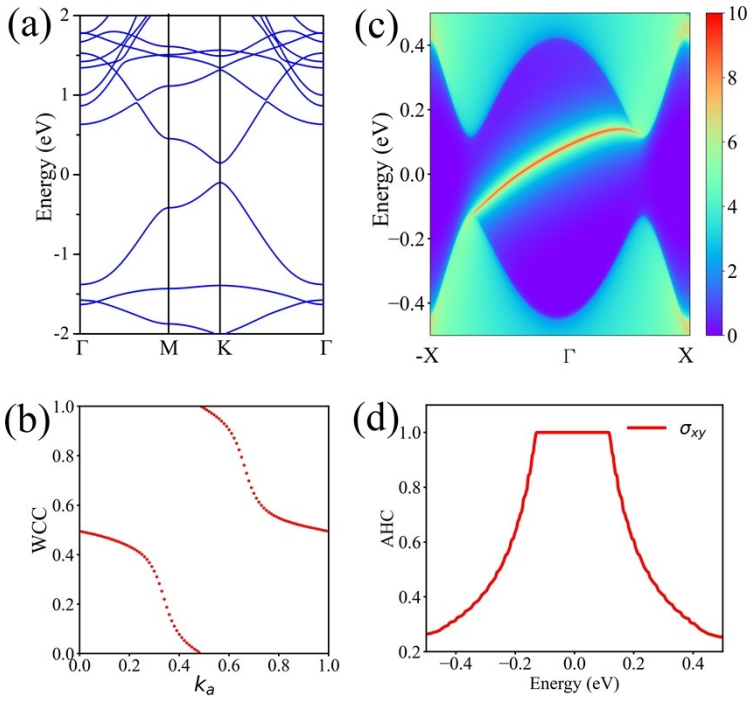

Fig. S1 (a) Band structure of Nb_2O_3 monolayer. (b) Topological edge states of Nb_2O_3 monolayer calculated along the (100) direction. (c) Evolution of the summed WCCs for Nb_2O_3 monolayer. (d) AHC with respect to the position of the Fermi level. All results are calculated from the hybrid functional (HSE06) method.

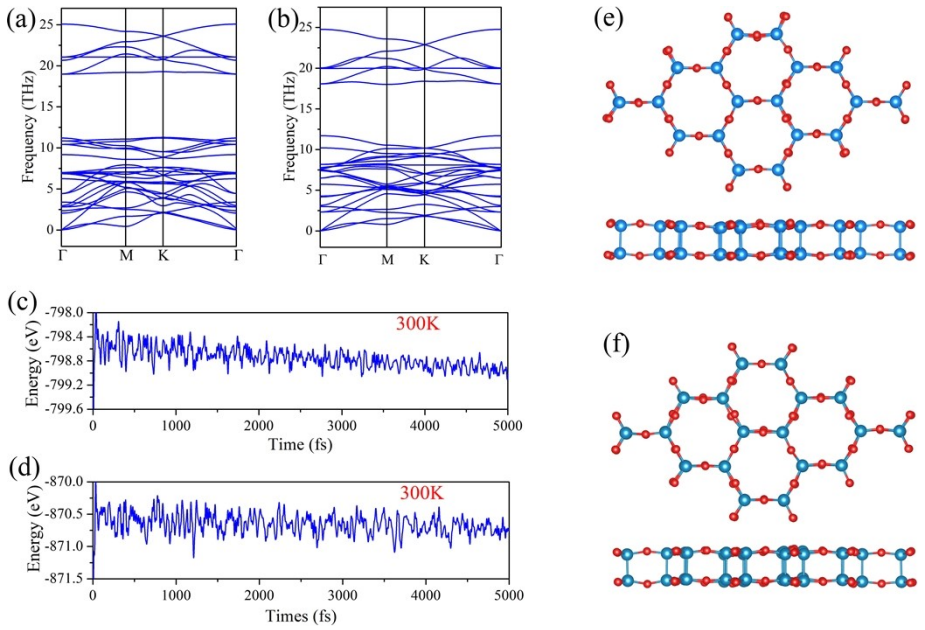

Fig. S2 Phonon dispersion of (a) Nb_2O_3 and (b) Ta_2O_3 bilayers. Total potential energy fluctuations of (c) Nb_2O_3 and (d) Ta_2O_3 bilayers during AIMD simulation at 300 K. The structures of (e) Nb_2O_3 and (f) Ta_2O_3 bilayers after 5 ps of AIMD simulation at 300 K.

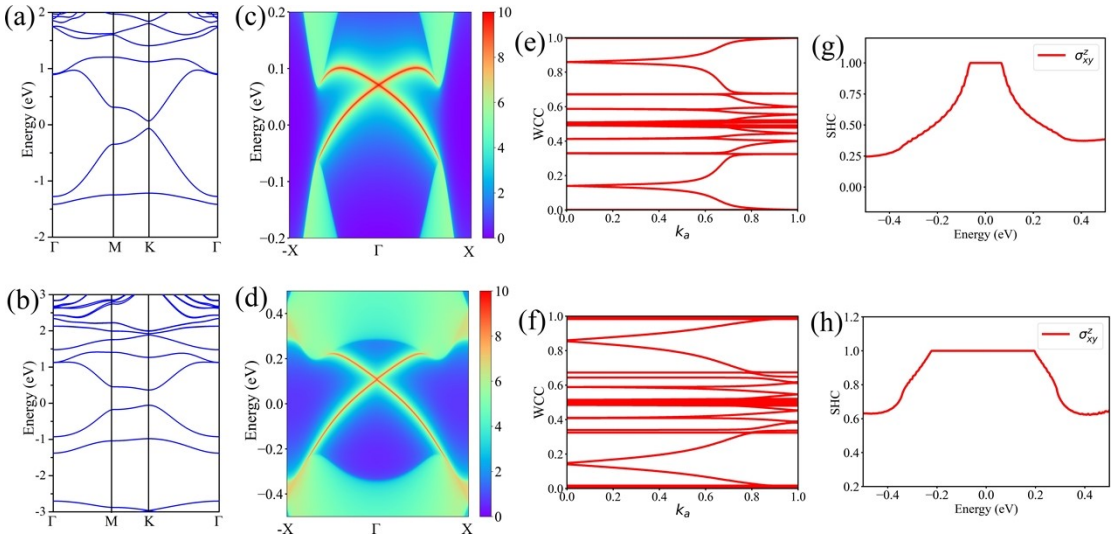

Fig. S3 Band structure of (a) Nb_2O_3 and (b) Ta_2O_3 bilayers. Topological edge states of (c) Nb_2O_3 and (d) Ta_2O_3 bilayers calculated along the (100) direction. WCCs of (e) Nb_2O_3 and (f) Ta_2O_3 bilayers. SHC of (g) Nb_2O_3 and (h) Ta_2O_3 bilayers. All results are calculated from the hybrid functional (HSE06) method.

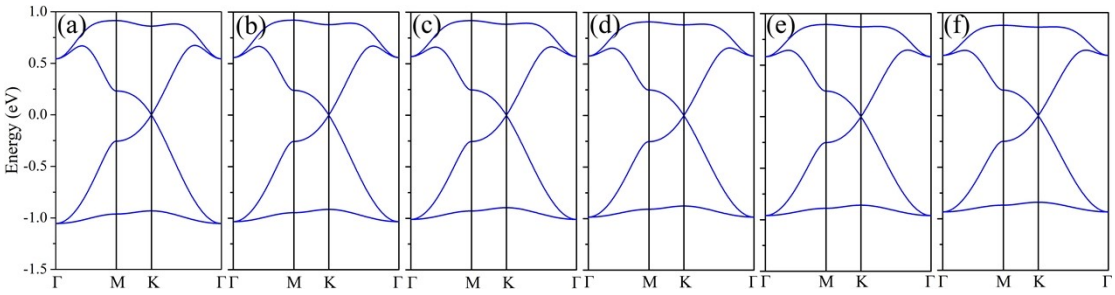

Fig. S4 Band structures of Nb_2O_3 bilayers in the strain range from 1% to 6%.

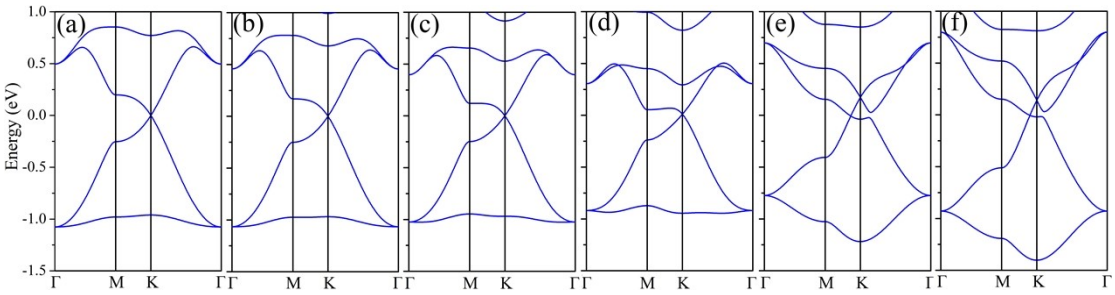

Fig. S5 Band structures of Nb_2O_3 bilayers in the strain range from -1% to -6%.

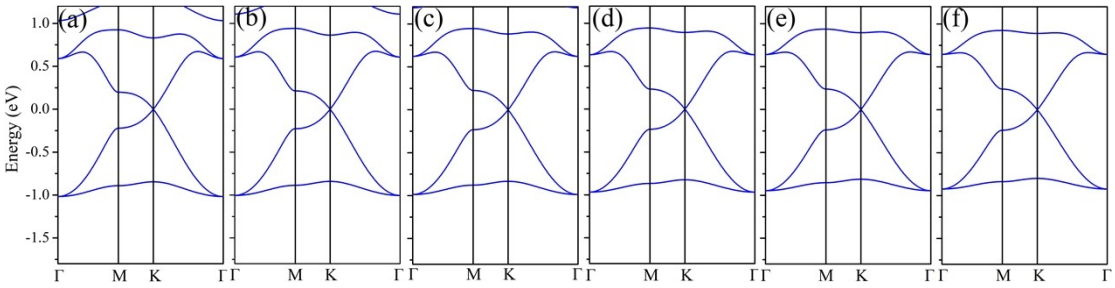

Fig. S6 Band structures of Ta_2O_3 bilayers in the strain range from 1% to 6%.

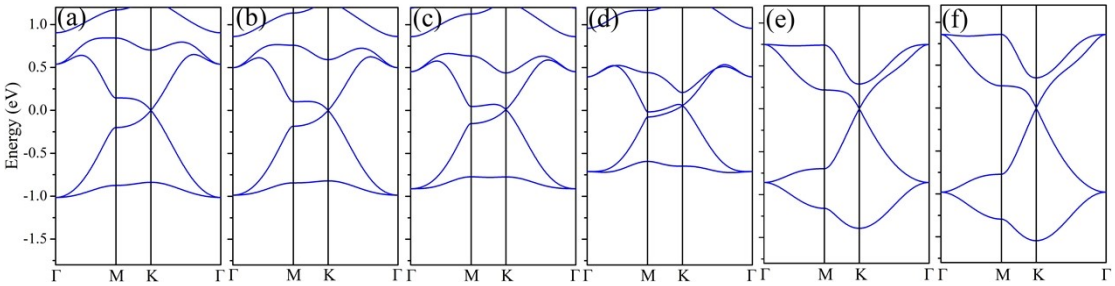

Fig. S7 Band structures of Ta_2O_3 bilayers in the strain range from -1% to -6%.

Table S1 Character table of the group D_{6h}.

$D_{6h}(6/mmm)$	#	1	6	3	2_z	2_{120}	2_{100}	-1	-6	-3	m_z	m_{120}	m_{100}	functions
Mult.	-	1	2	2	1	3	3	1	2	2	1	3	3	-
A_{1g}	Γ_1^+	1	1	1	1	1	1	1	1	1	1	1	1	x^2+y^2, z^2
A_{1u}	Γ_1^-	1	1	1	1	1	1	-1	-1	-1	1	-1	-1	.
A_{2g}	Γ_2^+	1	1	1	1	-1	-1	1	1	1	-1	-1	-1	J_z
A_{2u}	Γ_2^-	1	1	1	1	-1	-1	-1	-1	-1	1	1	1	z
B_{1g}	Γ_3^+	1	-1	1	-1	1	-1	1	-1	1	-1	1	-1	.
B_{1u}	Γ_3^-	1	-1	1	-1	1	-1	-1	1	-1	1	-1	1	.
B_{2g}	Γ_4^+	1	-1	1	-1	-1	1	1	-1	1	-1	-1	1	.
B_{2u}	Γ_4^-	1	-1	1	-1	-1	1	-1	1	-1	1	1	-1	.
E_{2u}	Γ_6^-	2	-1	-1	2	0	0	-2	1	1	-2	0	0	.
E_{2g}	Γ_6^+	2	-1	-1	2	0	0	2	-1	-1	2	0	0	(x^2-y^2, xy)
E_{1u}	Γ_5^-	2	1	-1	-2	0	0	-2	-1	1	2	0	0	(x, y)
E_{1g}	Γ_5^+	2	1	-1	-2	0	0	2	1	-1	-2	0	0	(xz,yz), (J_x,J_y)