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Single-layer $ZnMN_2$ (M=Si, Ge, Sn) zinc nitrides as promising photocatalysts

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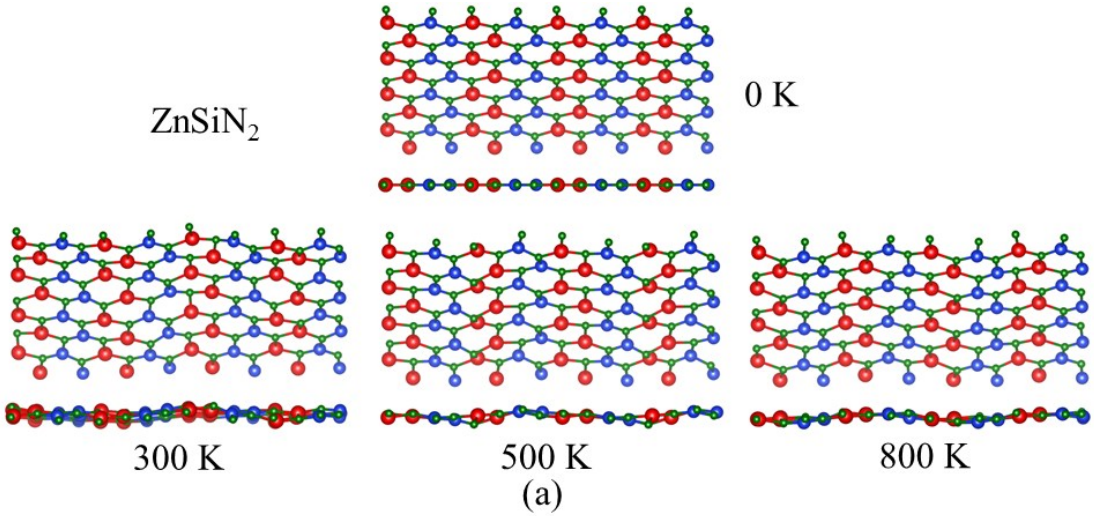
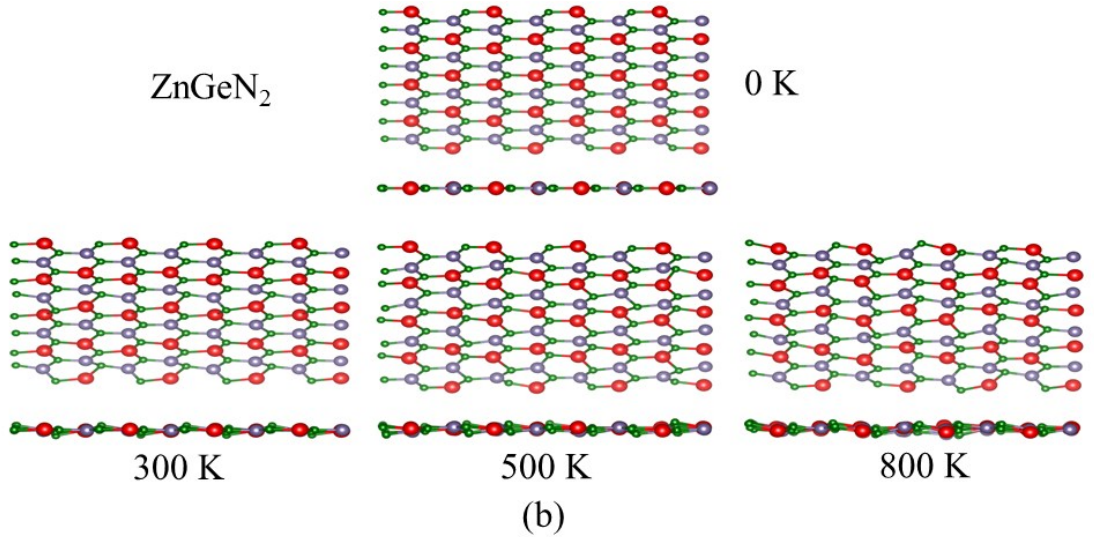
Table S1. Average bond lengths (in Å) of bulk and single-layer $ZnMN_2$ zinc nitrides.

Bulk	Zn-N	M-N	Single-layer	Zn-N	M-N
$ZnSiN_2$	2.06	1.76	$ZnSiN_2$	1.97	1.67
$ZnGeN_2$	2.06	1.89	$ZnGeN_2$	1.95	1.81
$ZnSnN_2$	2.08	2.09	$ZnSnN_2$	1.95	2.00



(a)



(b)

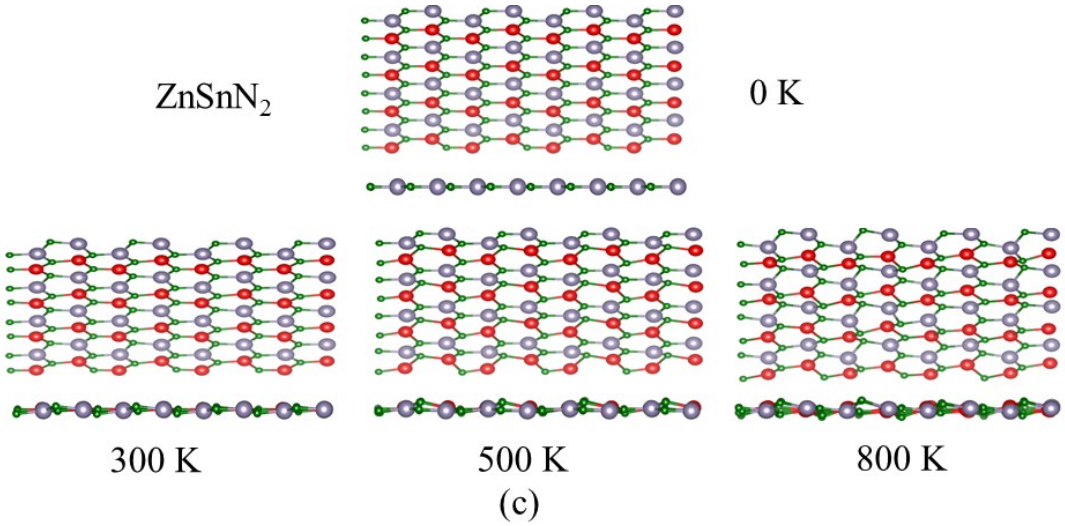


Fig. S1 Top and side views of the initial and final structures after first-principles molecular dynamics simulation at 300K, 500K and 800 K.

Table S2. The zero point energy corrections and entropic contributions to free energies at 298 K. The unit for energy is eV.

Species	TS	ZPE
H2O	0.67	0.56
H2	0.41	0.27
*O	0.00	0.05
*OH	0.00	0.35
*OOH	0.00	0.41