Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplemental Material for: Temperature-driven phase transition of Ti_2CN from first-principles calculations

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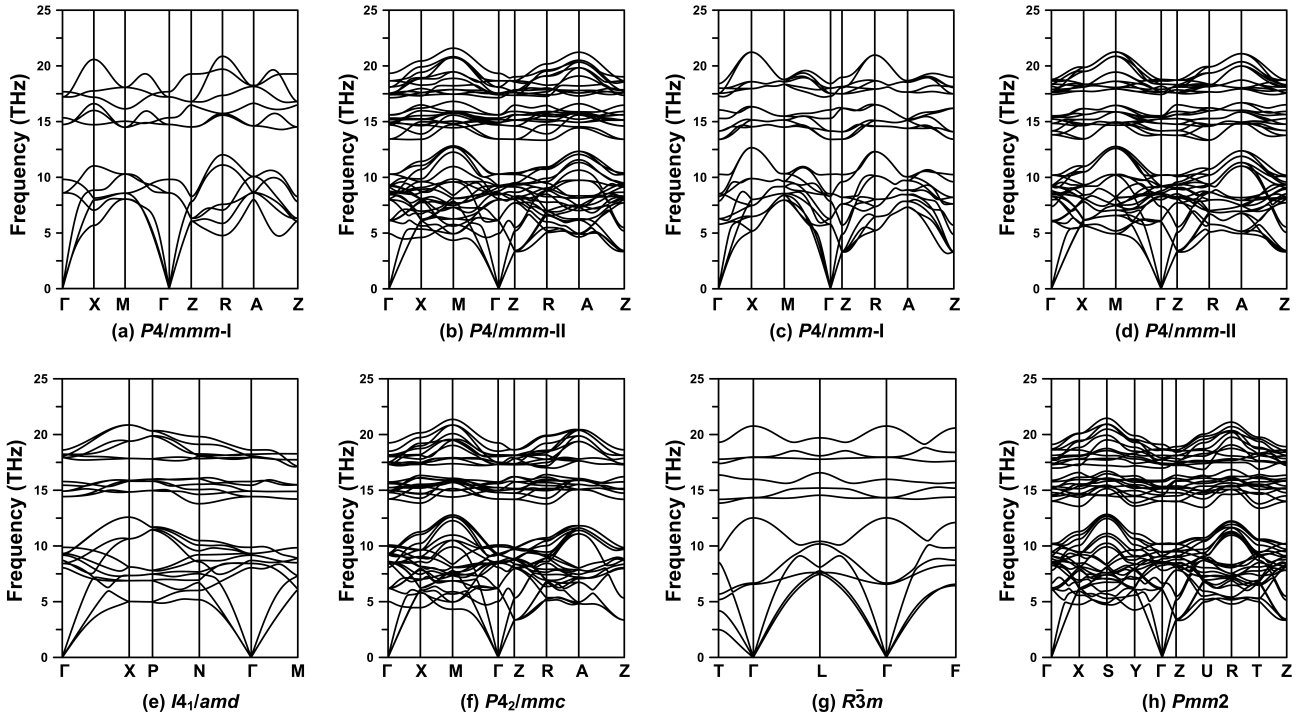

FIG. S1: Calculated phonon dispersion curves of Ti_2CN phases.

TABLE S1: Structural parameters of predicted Ti_2CN phases.

Structure type	Lattice constants	Wyckoff positions	x	y	z
$P4/mmm$-I	a=3.032	Ti 1b	0.000	0.000	0.500
	c=4.291	Ti 1c	0.500	0.500	0.000
		C 1a	0.000	0.000	0.000
		N 1d	0.500	0.500	0.500
$P4/mmm$-II	a=4.290	Ti 1b	0.000	0.000	0.500
	c=8.587	Ti 1a	0.000	0.000	0.000
		Ti 4i	0.500	0.000	0.248
		Ti 1c	0.500	0.500	0.000
		Ti 1d	0.500	0.500	0.500
		C 2f	0.000	0.500	0.000
		C 2g	0.000	0.000	0.252
		N 2h	0.500	0.500	0.747
		N 2e	0.500	0.000	0.500
$P4/nmm$-I	a=3.032	Ti 2c	0.500	0.000	0.870
	c=8.6034	Ti 2c	0.500	0.000	0.376
		C 2c	0.500	0.000	0.123
		N 2c	0.000	0.500	0.372
$P4/nmm$-II	a=4.2856	Ti 2c	0.000	0.500	0.496
	c=8.6073	Ti 2c	0.000	0.500	0.000
		Ti 4f	0.500	0.500	0.253
		C 1d	0.000	0.500	0.247
		C 1d	0.000	0.000	0.000
		N 1d	0.500	0.500	0.500
		N 1d	0.500	0.000	0.253
$I4_1/amd$	a=4.2848	Ti 8e	0.500	0.000	0.498
	c=8.6053	C 4a	0.000	0.000	0.000
		N 4b	0.500	0.500	0.000
$P4_2/mmc$	a=4.2874	Ti 2a	0.000	0.000	0.500
	c=8.5901	Ti 4i	0.500	0.000	0.252
		Ti 2b	0.500	0.500	0.000
		C 2c	0.000	0.500	0.000
		C 2e	0.000	0.000	0.250
		N 2d	0.500	0.000	0.000
		N 2f	0.500	0.500	0.750
$R\bar{3}m$	a=3.0316	Ti 6c	0.000	0.000	0.749
	c=14.9017	C 3a	0.000	0.000	0.000
		N 3b	0.667	0.333	0.833
$Pmm2$	a=4.2878	Ti 1c	0.500	0.000	0.499
	b=4.2884	Ti 1c	0.500	0.000	0.001
	c=8.5909	Ti 1d	0.500	0.500	0.750
		Ti 1d	0.500	0.500	0.249
		Ti 1a	0.000	0.000	0.755
		Ti 1a	0.000	0.000	0.247
		Ti 1b	0.000	0.500	0.497
		Ti 1b	0.000	0.500	0.251
		C 1d	0.500	0.500	0.999
		C 1d	0.500	0.500	0.501
		C 1a	0.000	0.000	0.999
		C 1b	0.000	0.500	0.251
		N 1c	0.500	0.000	0.748
		N 1c	0.500	0.000	0.252
		N 1a	0.000	0.000	0.502
		N 2b	0.000	0.500	0.749