Electronic Supplementary Material (ESI) for Nanoscale.

Supplementary information

Insights into regularity of 2D 3*d* transition metal monocarbides formation

K.V. Larionov[1,2], G. Seifert,[3] P.B. Sorokin[1,2]*

[1] National University of Science and Technology MISiS, 4 Leninskiy prospekt, Moscow, 119049, Russian Federation

[2] Moscow Institute of Physics and Technology, Institute lane 9, Dolgoprudniy, Moscow region, Russia

[3] Technische Universitaet Dresden, Bergstr. 66b, Dresden, Germany

* konstantin.larionov@phystech.edu

Table S1. Summarized data on the energy of 3*d* metal monocarbides in the case of different lattice and magnetic configuration. All number are presented in eV per one TM-C pair. Empty cells mean that corresponding state was not found.

TMC	Lattice	NM	FM	AFM1	AFM2	AFM3
ScC	*o*-	-	-	-	-	-
	t-	-14.29	-	-	-	-
	s-	-13.99	-	-	-	-
	g-	-13.22	-	-	-	-
TiC	*o*-	-15.80	-15.86	-15.80	-15.80	-15.81
	t-	-16.35	-	-	-	-
	s-	-16.23	-	-	-	-
	g-	-15.40	-	-	-	-
VC	*o*-	-16.75	-	-	-	-
	t-	-17.34	-	-	-17.34	-
	s-	-16.92	-16.95	-	-16.96	-
	g-	-15.68	-15.90	-15.86	-	-
CrC	*o*-	-17.07	-17.10	-17.43	-17.21	-17.27
	t-	-17.36	-17.48	-17.38	-	-17.41
	s-	-16.81	-17.28	-	-17.20	-
	g-	-15.80	-16.40	-16.14	-	-
MnC	*o*-	-16.61	-16.92	-16.90	-16.97	-16.99
	t-	-16.96	-17.09	-16.99	-	-17.01
	s-	-16.27	-16.51	-16.24	-16.38	-
	g-	-	-15.90	-	-	-
FeC	*o*-	-15.83	-16.13	-16.05	-16.05	-15.92
	t-	-16.16	-	-	-	-
	s-	-15.31	-15.30	-	-15.33	-
	g-	-14.98	-	-14.99	-	-
CoC	*o*-	-14.90	-14.91	-	-14.94	-
	t-	-14.76	-	-	-	-
	s-	-14.19	-	-	-	-
	g-	-13.69	-	-	-	-
NiC	*o*-	-13.49	-13.49	-	-	-
	t-	-12.44	-	-	-	-
	s-	-12.21	-	-	-	-
	g-	-	-	-	-	-
CuC	*o*-	-11.47	-	-	-	-
	t-	-9.37	-	-	-	-
	s-	-9.20	-	-	-	-
	g-	-	-	-	-	-

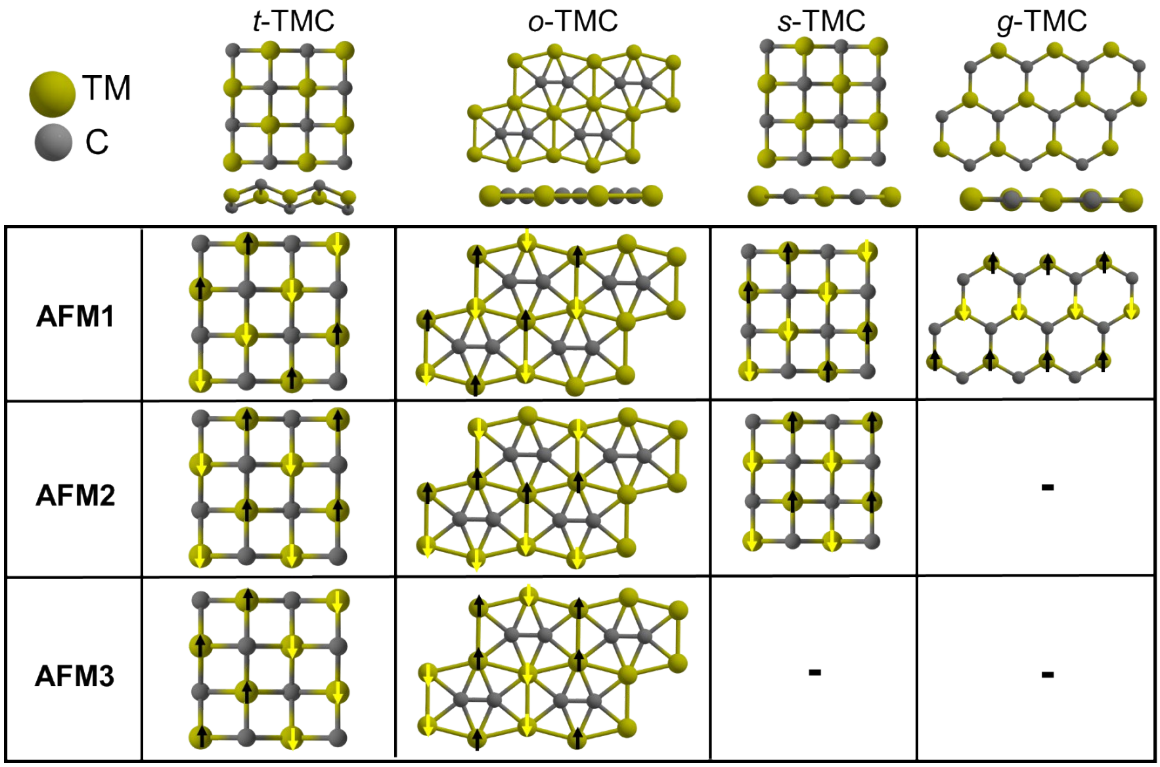

Figure S1. Possible antiferromagnetic configurations of *t*-TMC, *o*-TMC, *s*-TMC, and *g*-TMC, considered in Table S1.

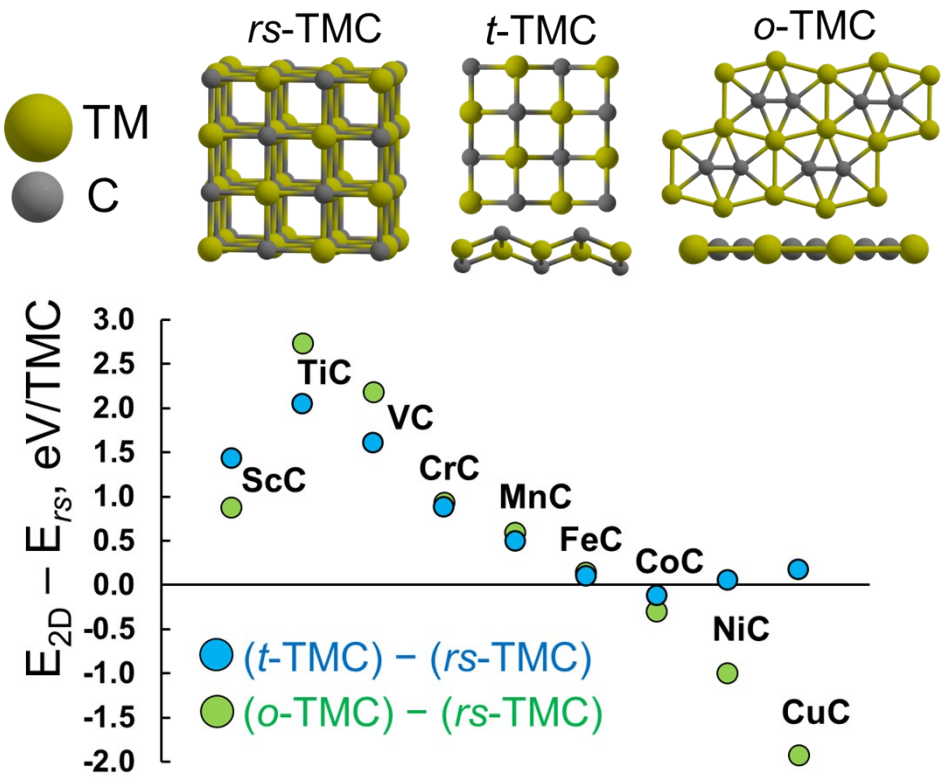

Figure S2. Calculated energy difference between *rs* bulk and 2D TMC phase: *t*-TMC or *o*-TMC shown by blue and green points, respectively. The structures of bulk *rs*-TMC, 2D *t*-TMC and *o*-TMC phases are shown above, where olive and grey spheres correspond to transition metal and carbon atoms, respectively.

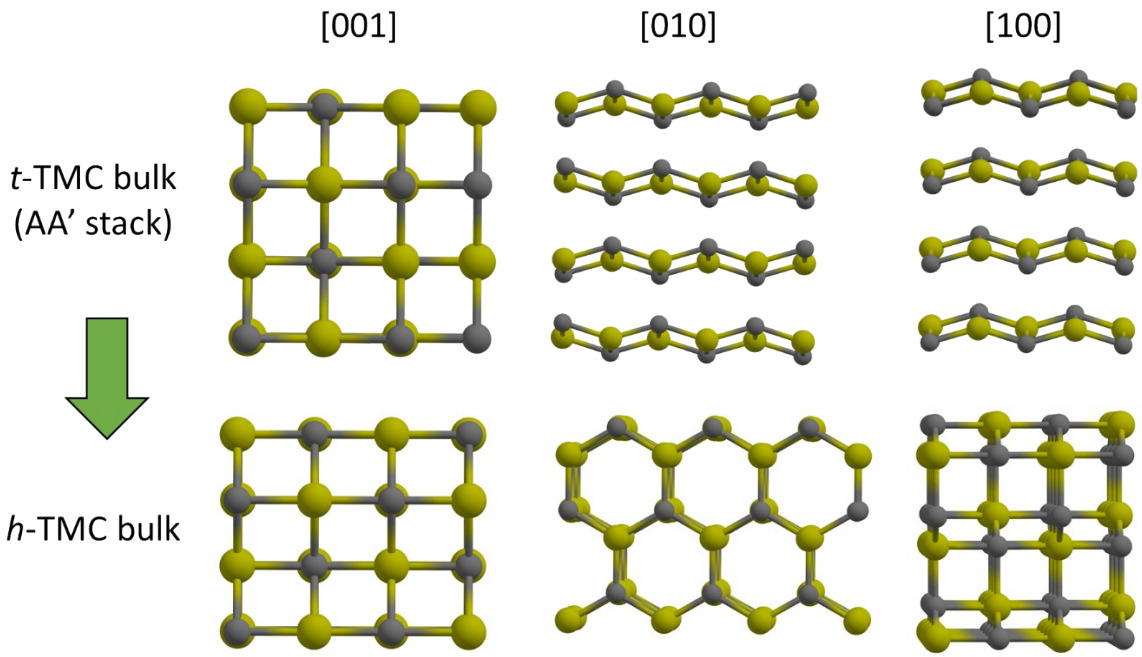

Figure S3. Views on different crystal directions of *t*-TMC bulk crystal (represented as AA' stack of separate *t*-TMC monolayers, see top row) and hexagonal-like *h*-TMC phase (see bottom row).

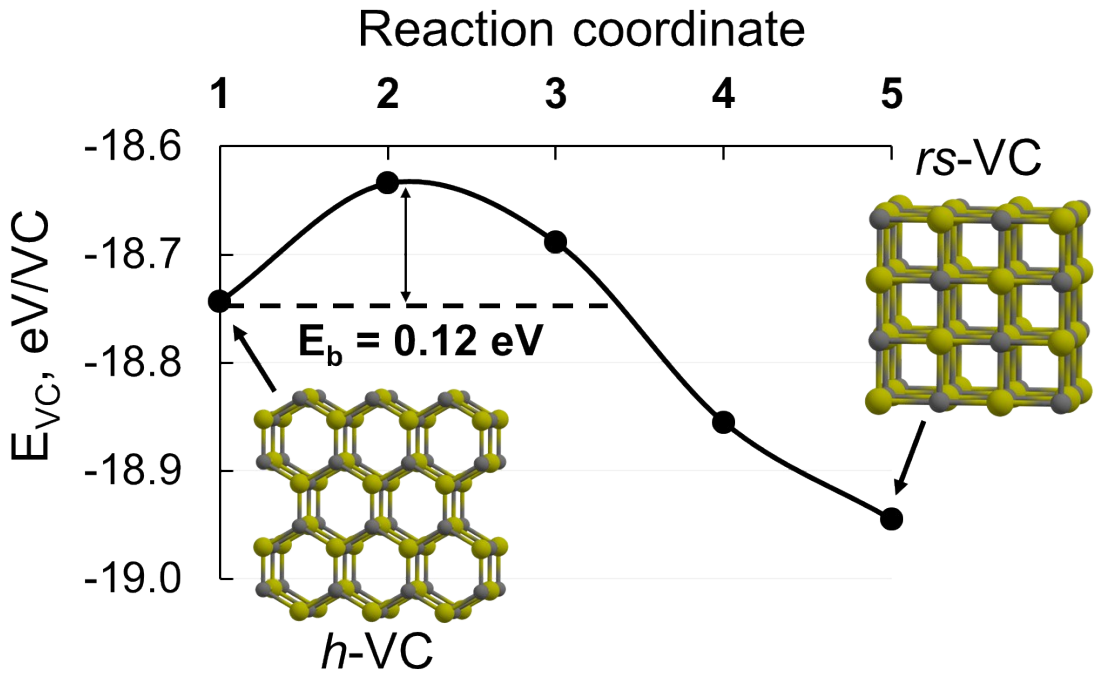

Figure S4. Transition pathway of VC monocarbide through a barrier, E_b, from hexagonal-like *h*-VC phase to energy favorable rocksalt (*rs*-VC) phase.

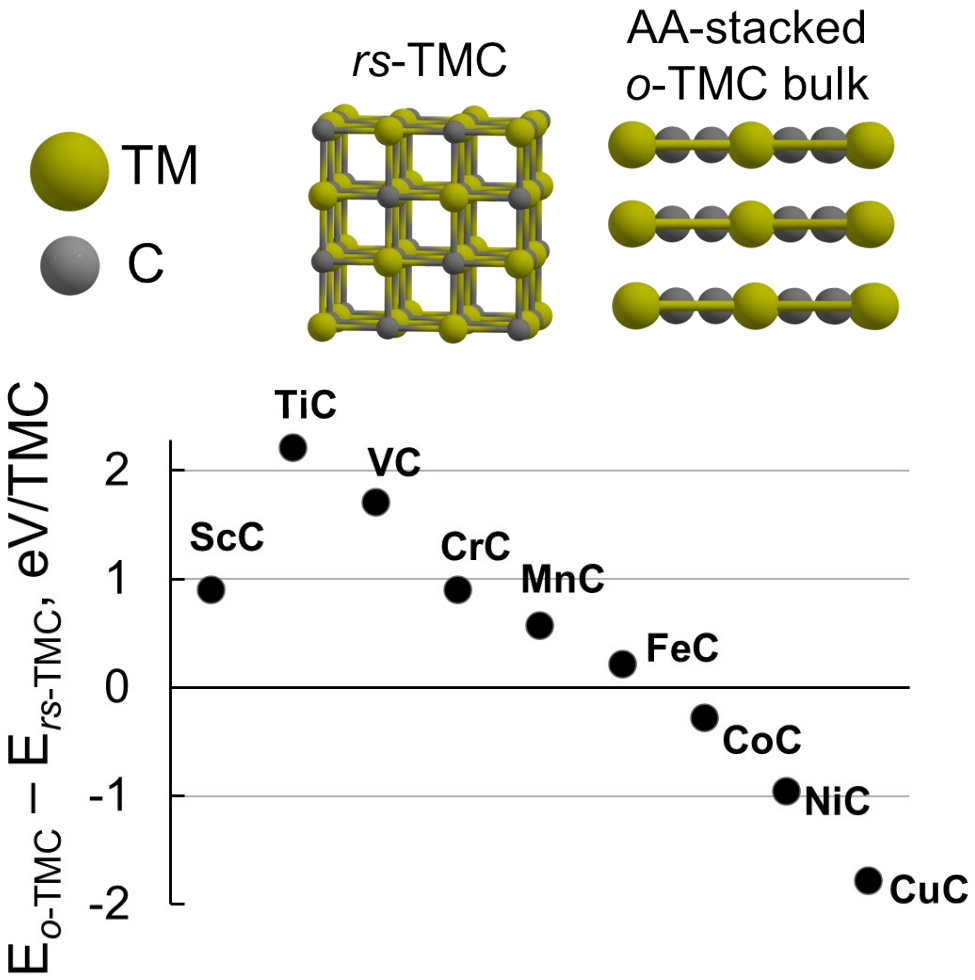

Figure S5. Calculated energy difference between proposed bulk phase consisted of AA stack of weakly bounded *o*-TMC monolayers ($E_{o\text{-TMC}}$) and rocksalt ($E_{rs\text{-TMC}}$) phase. Side views on their atomic structure are presented on the top, where olive and grey spheres correspond to transition metal and carbon atoms, respectively.