Diversity of Adsorbed Hydrogen on the TiC (001) Surface at High Coverages

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Figure S1 Top view of the TiC(001) surface. The image show C atoms (black), Ti atoms (blue), and H atom (pink) in the six initials positions under study. Top metal (M-top, 1), Top carbon (C-top, 2), Bridge between vicinal carbon and metal atoms (3), 4-fold hollow (4), 3-fold hollow formed by two metal and one carbon atoms (MMC, 5), and 3-fold hollow formed by two carbon and one metal atoms (CCM, 6).

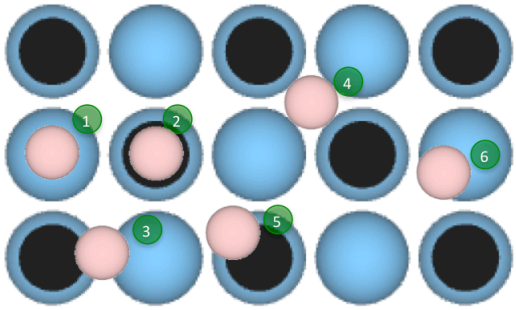

Table S1. Adsorption energies of an H atom on the TiC(001) surface. Values are given in eV.

TiC	M-top	C-top	CCM
PBE	-0.73	-2.73	-1.77
PBE-D3	-0.83	-2.83	-1.89

Figure S2. Top view of the TiC(001) surface. The image shows C atoms (black), Ti atoms (blue), and H_2 molecule (pink) in the 19 initial positions under study. Positions 1 to 6 correspond to a vertical orientation of the H_2 molecule and positions 7 to 19 correspond to horizontal orientation of the of the H_2 molecule. Dashed orange lines are guides to the eyes.

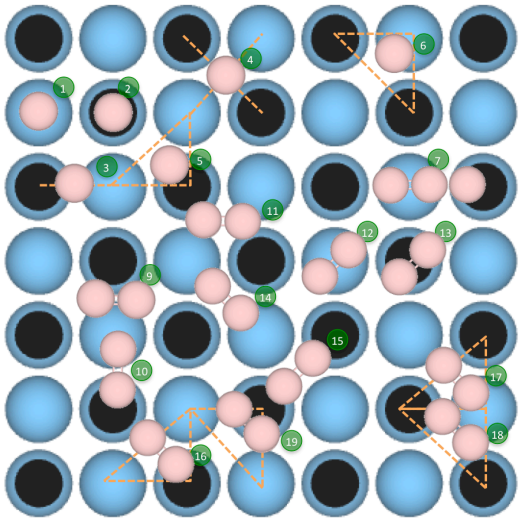

Tabla S2. H_2 adsorption energies on the TiC(001) surface. All values are given in eV.

Position	1	7	8	10	12	13
PBE	-0.07	-0.07	-0.23	-0.07	-0.07	-0.46
PBE-D3	-0.21	-0.21	-0.41	-0.21	-0.20	-0.66

Figure S3. Top view of the H atom addition sequence on C-top sites on the TiC(001) surface.

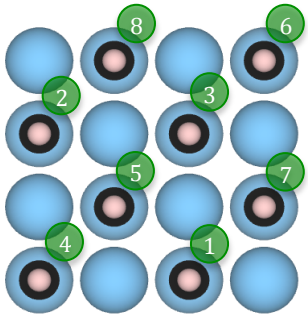

Table S3. Adsorption energies (E_{ads}, in eV) for different H atom coverages on the TiC (001) surface.

H atoms	1	2	3	4	5	6	7	8
PBE	-2.73	-2.71	-2.47	-2.36	-2.49	-2.30	-2.11	-1.94
PBE-D3	-2.83	-2.81	-2.64	-2.61	-2.61	-2.41	-2.21	-2.02

Table S4. Adsorption energies (E_{ads}, in eV) for different H atoms coverages on the TiC (001) surface using $^1/_2 \cdot H_2$ molecule as reference.

H atoms	1	2	3	4	5	6	7	8
PBE	-0.47	-0.44	-0.20	-0.10	-0.23	-0.03	0.15	0.33
PBE-D3	-0.56	-0.54	-0.29	-0.19	-0.35	-0.14	0.05	0.24