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Correction: Two-dimensional nitrides as highly efficient potential candidates for CO₂ capture and activation

Raul Morales-Salvador, Ángel Morales-García, Francesc Viñes and Francesc Illas*

Correction for 'Two-dimensional nitrides as highly efficient potential candidates for CO₂ capture and activation' by Raul Morales-Salvador *et al.*, *Phys. Chem. Chem. Phys.*, 2018, **20**, 17117–17124.

The authors would like to correct errors associated with the reported PBE calculations. Due to a problem in the backup of some of the output files, the reported PBE results for the clean surfaces do not correspond to the fully relaxed structure. Once the proper energies are used, the E_{ads} (PBE) values become on average 0.34 eV larger thus favoring adsorption. This implies that E_{ads} (PBE-D3) values are larger than PBE ones by 0.30 eV and not 0.7–1.0 eV as reported in *Phys. Chem. Chem. Phys.*, 2018, **20**, 17117–17124. As a consequence, desorption temperatures predicted by the PBE calculations need to be corrected becoming higher.

The error found in the set of PBE results does not affect the main conclusion of the manuscript based on the more accurate PBE-D3 method indicating that 2D nitrides are potential materials for the capture and activation of CO₂. Updated versions of Fig. 2 and Tables S1 and S3 are included.

Fig. 2 (a) Calculated rates for desorption and adsorption of CO_2 on Ta_2N and $Ti_2N(0001)$ surfaces. On Ta_2N marked points with T_1 – T_6 labels show how desorption temperature ranges, in (b), have been obtained. In (a), green, gray and blue colors correspond to adsorption rates on a single site per time unit for a CO_2 partial pressure of 40, 15×10^3 , and 10^5 Pa, respectively. Black and red lines are desorption rates per site for E_{ads} obtained from PBE (solid) and PBE-D3 (dashed) calculations. In (b), green, gray, and blue bars belong to desorption temperature ranges for CO_2 partial pressures of 40, 15×10^3 , and 10^5 Pa, respectively.

Table S1 Adsorption energy (in eV) of CO₂ molecule on MXene carbides at PBE and PBE-D3 levels on the adsorption sites described in Fig 1. Bond lengths $\delta(\text{CO})$ and $\delta(\text{MO})$ are given in Å, as well as the CO₂ molecular angle, $\alpha(\text{OCO})$, in degrees. The Bader charge analysis, ΔQ , is given in e and corresponds to charge difference between the adsorbed and isolated CO₂ molecule

MXene	Level	E_{ads}^a	$\delta(\text{MO})$	$\delta(\text{CO})$	$\alpha(\text{OCO})$	ΔQ
$\eta^1\text{-CO}_2\text{-}\mu^2\text{-C}_\text{B}$						
Cr ₂ N	PBE	−0.98	2.10 (×2)	1.26 (×2)	136.8	−0.89
	PBE-D3	−1.30	2.10 (×2)	1.26 (×2)	136.8	−0.90
Hf ₂ N	PBE	−2.16	2.18 (×2)	1.29 (×2)	130.1	−1.47
	PBE-D3	−2.29	2.18 (×2)	1.29 (×2)	129.9	−1.47
Nb ₂ N	PBE	−1.42	2.24 (×2)	1.27 (×2)	132.6	−1.11
	PBE-D3	−1.73	2.23 (×2)	1.27 (×2)	132.4	−1.12
Ta ₂ N	PBE	−1.62	2.16 (×2)	1.28 (×2)	132.4	−1.20
	PBE-D3	−1.90	2.16 (×2)	1.28 (×2)	132.4	−1.21
V ₂ N	PBE	−1.39	2.11 (×2)	1.27 (×2)	134.6	−1.08
	PBE-D3	−1.67	2.10 (×2)	1.27 (×2)	134.6	−1.08
Mo ₂ N	PBE	−0.98	2.24 (×2)	1.26 (×2)	136.2	−1.06
	PBE-D3	−1.33	2.23 (×2)	1.26 (×2)	136.2	−1.06
W ₂ N	PBE	−0.76	2.22 (×2)	1.26 (×2)	136.8	−0.86
	PBE-D3	−1.21	2.22 (×2)	1.26 (×2)	136.7	−0.86
$\eta^2\text{-CO}_2\text{-}\mu^3\text{-C}_\text{M}\text{O}_\text{B}$						
Nb ₂ N	PBE	−1.38	2.40;2.39	1.26;1.33	130.8	−1.35
	PBE-D3	−1.69	2.39 (×2)	1.26;1.33	130.9	−1.35
V ₂ N	PBE	−1.36	2.25;2.24	1.26;1.32	133.1	−1.30
	PBE-D3	−1.65	2.23;2.25	1.26;1.32	133.1	−1.30
Mo ₂ N	PBE	−0.68	2.36;2.36	1.26;1.30	134.7	−1.39
	PBE-D3	−1.03	2.35;2.36	1.26;1.30	134.7	−1.39
$\eta^2\text{-CO}_2\text{-}\mu^3\text{-C}_\text{N}\text{O}_\text{B}$						
Cr ₂ N	PBE	−0.88	2.22;2.18	1.25;1.31	135.0	−1.12
	PBE-D3	−1.21	2.22;2.17	1.25;1.31	135.0	−1.14
Nb ₂ N	PBE	−1.18	2.39;2.36	1.26;1.33	132.1	−1.34
	PBE-D3	−1.50	2.39;2.36	1.26;1.33	132.2	−1.35
V ₂ N	PBE	−1.21	2.26;2.21	1.26;1.32	133.9	−1.32
	PBE-D3	−1.51	2.25;2.21	1.26;1.33	134.0	−1.32
$\eta^3\text{-CO}_2\text{-}\mu^5\text{-C}_\text{M}\text{O}_\text{N}\text{O}_\text{N}$						
Zr ₂ N	PBE	−2.72	2.34;2.352.34;2.35	1.36 (×2)	116.2	−1.79
	PBE-D3	−2.83	2.34;2.352.34;2.35	1.36;1.37	116.2	−1.80
Hf ₂ N	PBE	−2.82	2.32;2.33	1.35;1.44	114.0	−2.02
	PBE-D3	−2.97	2.22;2.33	1.35;1.44	114.0	−2.02
Ti ₂ N	PBE	−2.92	2.23 (×2)	1.40;1.36	115.9	−1.86
	PBE-D3	−3.13	2.23;2.192.23;2.16	1.40;1.36	115.9	−1.87
$\eta^3\text{-CO}_2\text{-}\mu^5\text{-C}_\text{N}\text{O}_\text{M}\text{O}_\text{M}$						
Ta ₂ N	PBE	−1.60	2.00 (×2)	1.38 (×2)	112.8	−1.65
	PBE-D3	−1.89	2.00 (×2)	1.38 (×2)	112.8	−1.65
W ₂ N	PBE	−1.30	2.00 (×2)	1.37 (×2)	114.0	−1.40
	PBE-D3	−1.77	2.00 (×2)	1.37 (×2)	114.0	−1.40
Ti ₂ N	PBE	−2.92	2.20;2.14(×2)	1.39;1.40	115.3	−1.94
	PBE-D3	−3.13	2.20;2.13(×2)	1.39;1.40	115.2	−1.94
$\eta^2\text{-CO}_2\text{-}\mu^4\text{-O}_\text{B}\text{O}_\text{B}$						
Ta ₂ N	PBE	−0.30	2.10;2.30(×2)	1.39 (×2)	106.8	−1.62
	PBE-D3	−0.61	2.10;2.31(×2)	1.39 (×2)	106.8	−1.63
$\eta^3\text{-CO}_2\text{-}\mu^4\text{-C}_\text{B}\text{O}_\text{B}\text{O}_\text{B}$						
Mo ₂ N	PBE	−0.98	2.22;2.282.19;2.31	1.38;1.36	111.2	−1.81
	PBE-D3	−1.34	2.22;2.282.19;2.31	1.38;1.36	111.2	−1.82
Cr ₂ N	PBE	−1.08	2.09;1.982.05;2.25	1.39;1.29	121.3	−1.27
	PBE-D3	−1.44	2.08;1.972.05;2.25	1.39;1.29	121.3	−1.28
$\eta^3\text{-CO}_2\text{-}\mu^4\text{-C}_\text{M}\text{O}_\text{M}\text{O}_\text{B}$						
W ₂ N	PBE	−2.20	2.17;2.04	1.33;1.39	116.5	−1.41
	PBE-D3	−2.59	2.17;2.04	1.33;1.39	116.5	−1.41

^a ZPE corrected as above stated.

Table S3 Desorption temperature range ([PBE]–[PBE-D3]) for CO₂ partial pressure ranges for CO₂ partial pressures of 40, 15 × 10³, and 10⁵ Pa, which stand for air, exhaust, and desorption situations, respectively. All temperature values are given in K

MXene	Temperature range		
	Air	Exhaust	Desorption
$\eta^1\text{-CO}_2\text{-}\mu^2\text{-C}_\text{B}$			
Cr ₂ N	415–548	529–704	581–776
Hf ₂ N	946–1004	1237–1316	1373–1463
Nb ₂ N	607–741	782–958	864–1060
Ta ₂ N	669–784	853–1004	937–1104
V ₂ N	594–715	765–924	844–1023
Mo ₂ N	412–559	526–718	577–791
W ₂ N	314–498	395–634	433–696
$\eta^2\text{-CO}_2\text{-}\mu^3\text{-C}_\text{MO}_\text{B}$			
Nb ₂ N	591–726	763–938	842–1037
V ₂ N	603–730	786–952	871–1057
Mo ₂ N	302–453	389–586	428–648
$\eta^2\text{-CO}_2\text{-}\mu^3\text{-C}_\text{NO}_\text{B}$			
Cr ₂ N	383–523	489–672	538–741
Nb ₂ N	517–650	666–843	736–934
V ₂ N	535–661	692–859	764–949
$\eta^3\text{-CO}_2\text{-}\mu^5\text{-C}_\text{MON}_\text{O}_\text{N}$			
Zr ₂ N	1150–1199	1484–1549	1639–1712
Hf ₂ N	1138–1261	1449–1631	1591–1804
Ti ₂ N	1239–1338	1603–1735	1772–1921
$\eta^3\text{-CO}_2\text{-}\mu^5\text{-C}_\text{NOM}_\text{OM}$			
Ta ₂ N	646–761	815–962	890–1053
W ₂ N	512–697	641–877	697–956
Ti ₂ N	1239–1339	1603–1736	1773–1922
$\eta^2\text{-CO}_2\text{-}\mu^4\text{-O}_\text{BO}_\text{B}$			
Ta ₂ N	152–276	191–344	205–377
$\eta^3\text{-CO}_2\text{-}\mu^4\text{-C}_\text{BO}_\text{BO}_\text{B}$			
Mo ₂ N	408–531	515–669	563–729
Cr ₂ N	444–579	560–734	611–803
$\eta^3\text{-CO}_2\text{-}\mu^4\text{-C}_\text{MOM}_\text{OB}$			
W ₂ N	872–1029	1102–1305	1205–1430

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