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# Correction: Two-dimensional nitrides as highly efficient potential candidates for $CO_2$ capture and activation

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Correction for 'Two-dimensional nitrides as highly efficient potential candidates for $CO_2$ 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 $CO_2$. Updated versions of Fig. 2 and Tables S1 and S3 are included.

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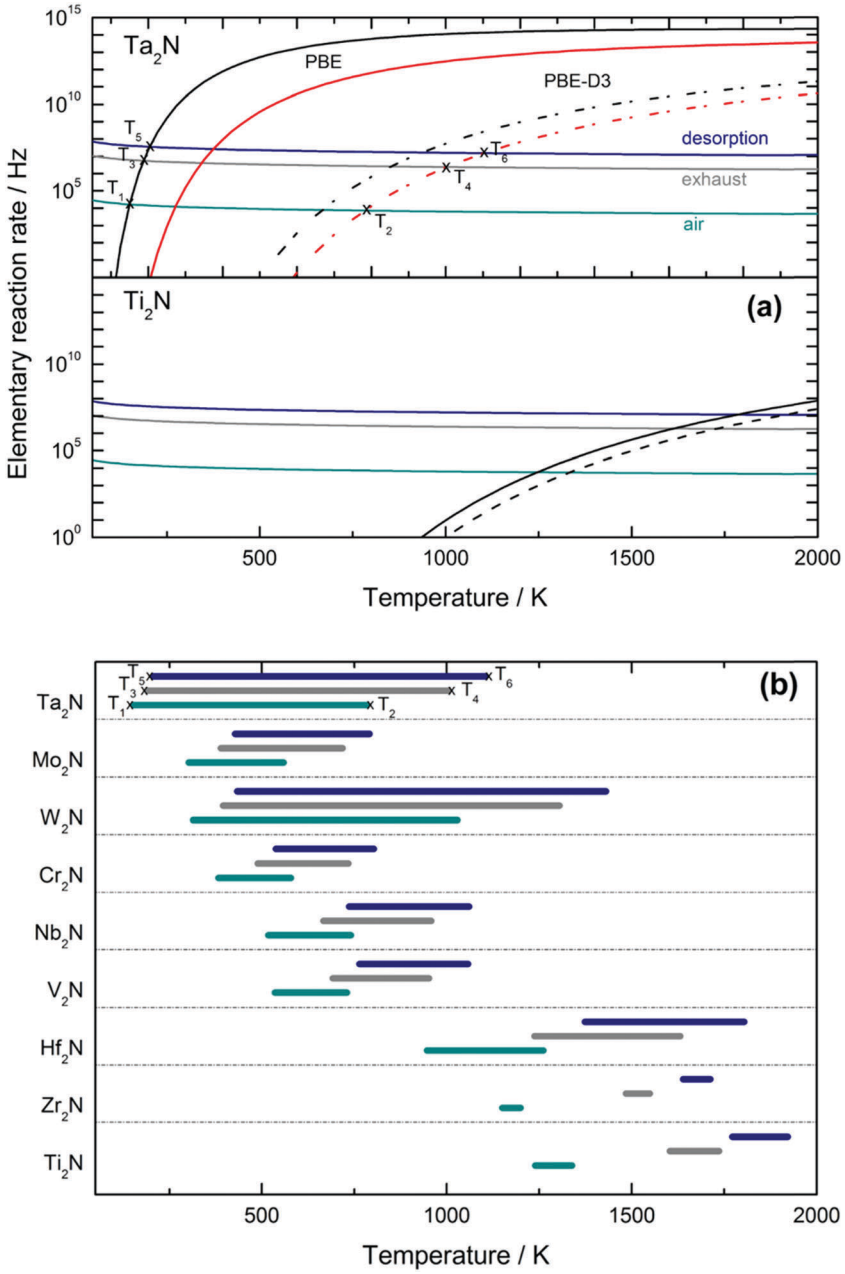


Fig. 2 (a) Calculated rates for desorption and adsorption of $CO_2$ on $Ta_2N$ and $Ti_2N(0001)$ surfaces. On $Ta_2N$ marked points with $T_1$–$T_6$ labels show how desorption temperature ranges, in (b), have been obtained. In (a), green, gray and blue colors correspond to adsorption rates on a single site per time unit for a $CO_2$ partial pressure of 40, $15 \times 10^3$, 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, $15 \times 10^3$, and $10^5$ Pa, respectively.

Table S1 Adsorption energy (in eV) of $CO_2$ molecule on MXene carbides at PBE and PBE-D3 levels on the adsorption sites described in Fig 1. Bond lengths $\delta$(CO) and $\delta$(MO) are given in Å, as well as the $CO_2$ molecular angle, $\alpha$(OCO), in degrees. The Bader charge analysis, $\Delta Q$, is given in $e$ and corresponds to charge difference between the adsorbed and isolated $CO_2$ molecule

| MXene | Level | $E_{ads}$[a] | $\delta$(MO) | $\delta$(CO) | $\alpha$(OCO) | $\Delta Q$ |
|---|---|---|---|---|---|---|
| | | | $\eta^1$-$CO_2$-$\mu^2$-$C_B$ | | | |
| $Cr_2N$ | 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 |
| $Hf_2N$ | 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 |
| $Nb_2N$ | 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 |
| $Ta_2N$ | 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 |
| $V_2N$ | 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 |
| $Mo_2N$ | 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 |
| $W_2N$ | 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 |
| | | | $\eta^2$-$CO_2$-$\mu^3$-$C_MO_B$ | | | |
| $Nb_2N$ | 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 |
| $V_2N$ | 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 |
| $Mo_2N$ | 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 |
| | | | $\eta^2$-$CO_2$-$\mu^3$-$C_NO_B$ | | | |
| $Cr_2N$ | 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 |
| $Nb_2N$ | 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 |
| $V_2N$ | 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 |
| | | | $\eta^3$-$CO_2$-$\mu^5$-$C_MO_NO_N$ | | | |
| $Zr_2N$ | 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 |
| $Hf_2N$ | 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 |
| $Ti_2N$ | 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 |
| | | | $\eta^3$-$CO_2$-$\mu^5$-$C_NO_MO_M$ | | | |
| $Ta_2N$ | 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 |
| $W_2N$ | 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 |
| $Ti_2N$ | 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 |
| | | | $\eta^2$-$CO_2$-$\mu^4$-$O_BO_B$ | | | |
| $Ta_2N$ | 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 |
| | | | $\eta^3$-$CO_2$-$\mu^4$-$C_BO_BO_B$ | | | |
| $Mo_2N$ | 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 |
| $Cr_2N$ | 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 |
| | | | $\eta^3$-$CO_2$-$\mu^4$-$C_MO_MO_B$ | | | |
| $W_2N$ | 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 $CO_2$ partial pressure ranges for $CO_2$ partial pressures of 40, $15 \times 10^3$, and $10^5$ Pa, which stand for air, exhaust, and desorption situations, respectively. All temperature values are given in K

| | Temperature range | | |
|---|---|---|---|
| MXene | Air | Exhaust | Desorption |
| **$\eta^1$-$CO_2$-$\mu^2$-$C_B$** | | | |
| $Cr_2N$ | 415–548 | 529–704 | 581–776 |
| $Hf_2N$ | 946–1004 | 1237–1316 | 1373–1463 |
| $Nb_2N$ | 607–741 | 782–958 | 864–1060 |
| $Ta_2N$ | 669–784 | 853–1004 | 937–1104 |
| $V_2N$ | 594–715 | 765–924 | 844–1023 |
| $Mo_2N$ | 412–559 | 526–718 | 577–791 |
| $W_2N$ | 314–498 | 395–634 | 433–696 |
| **$\eta^2$-$CO_2$-$\mu^3$-$C_MO_B$** | | | |
| $Nb_2N$ | 591–726 | 763–938 | 842–1037 |
| $V_2N$ | 603–730 | 786–952 | 871–1057 |
| $Mo_2N$ | 302–453 | 389–586 | 428–648 |
| **$\eta^2$-$CO_2$-$\mu^3$-$C_NO_B$** | | | |
| $Cr_2N$ | 383–523 | 489–672 | 538–741 |
| $Nb_2N$ | 517–650 | 666–843 | 736–934 |
| $V_2N$ | 535-661 | 692–859 | 764–949 |
| **$\eta^3$-$CO_2$-$\mu^5$-$C_MO_NO_N$** | | | |
| $Zr_2N$ | 1150–1199 | 1484–1549 | 1639–1712 |
| $Hf_2N$ | 1138–1261 | 1449–1631 | 1591–1804 |
| $Ti_2N$ | 1239–1338 | 1603–1735 | 1772–1921 |
| **$\eta^3$-$CO_2$-$\mu^5$-$C_NO_MO_M$** | | | |
| $Ta_2N$ | 646–761 | 815–962 | 890–1053 |
| $W_2N$ | 512–697 | 641–877 | 697–956 |
| $Ti_2N$ | 1239–1339 | 1603–1736 | 1773–1922 |
| **$\eta^2$-$CO_2$-$\mu^4$-$O_BO_B$** | | | |
| $Ta_2N$ | 152–276 | 191–344 | 205–377 |
| **$\eta^3$-$CO_2$-$\mu^4$-$C_BO_BO_B$** | | | |
| $Mo_2N$ | 408–531 | 515–669 | 563–729 |
| $Cr_2N$ | 444–579 | 560–734 | 611–803 |
| **$\eta^3$-$CO_2$-$\mu^4$-$C_MO_MO_B$** | | | |
| $W_2N$ | 872–1029 | 1102–1305 | 1205–1430 |

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