Supporting information of

Water adsorption on MO$_2$ (M = Ti, Ru and Ir) surfaces.

Importance of octahedral distortion and cooperative effects.

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Table S1: Adsorption energies for the single water adsorption on the TiO$_2$ (110) and (011) rutile surfaces. The relative energies ($\Delta E$) are calculated with respect to the water adsorbed in its molecular form (mol). The adsorption energies are calculated as $\Delta E_{ads} = E_{complex} - E_{surf} - E_{H2O}$, with each system optimized separately.

| (h k l) | Adsorption mode | PBE-D2 $\Delta E_{ads}$ (kJ/mol) | PBE-D3 $\Delta E$ (kJ/mol) | PBE0-D2 $\Delta E_{ads}$ (kJ/mol) | PBE0-D3 $\Delta E$ (kJ/mol) |
|--------|-----------------|-------------------------------|-----------------------------|-----------------------------------|-------------------------------|
| (110)  | mol             | -86.9                         | 0.0                         | -85.4                             | 0.0                           |
| (110)  | diss            | -52.2                         | 34.7                        | -47.7                             | 37.7                          |
| (011)  | mol             | -136.2                        | 0.0                         | -129.3                            | 0.0                           |
| (011)  | diss            | -140.0                        | -3.7                        | -134.5                            | -5.2                          |

Table S2: PBE-D2 adsorption energies for the single water adsorption on different TiO$_2$ (110) rutile surface models. The relative energies ($\Delta E$) are calculated with respect to the water adsorbed in its molecular form (mol). The adsorption energies are calculated as $\Delta E_{ads} = E_{complex} - E_{surf} - E_{H2O}$, with each system optimized separately.

| Number of layers | Adsorption mode | PBE-D2 $\Delta E$ (kJ mol$^{-1}$) | PBE-D2 $\Delta E_{ads}$ (kJ mol$^{-1}$) |
|------------------|-----------------|----------------------------------|--------------------------------------|
| 4 layer          | mol             | 0.0                              | -86.9                                |
|                  | diss            | 34.7                             | -52.2                                |
| 5 layer          | mol             | 0.0                              | -105.6                               |
|                  | diss            | -8.6                             | -114.3                               |
| 6 layer          | mol             | 0.0                              | -89.8                                |
|                  | diss            | 26.1                             | -63.6                                |
| 7 layer          | mol             | 0.0                              | -95.0                                |
|                  | diss            | 4.3                              | -90.6                                |
**Figure S1**: PBE-D2 calculated surface energies.

**Figure S2**: PBE-D2 geometries for the reconstructed (right) and non-reconstructed (left) TiO$_2$ (011) rutile surface.
**Figure S3**: Surface energy for the reconstructed (blue line) and non-reconstructed (green points) TiO$_2$ (011) rutile surface.

**Figure S4**: M—O$_w$ distances of two neighbor water adsorbed (in Å) along the dynamics.