Introduction
The project deals with the $H_2$ adsorption and dissociation into $H + H$ on the (001) surfaces of various transitions metal carbides (TMCs; TM=Ti, V, Zr, Nb, Mo, Hf, Ta), all displaying the NaCl crystalllographic structure.

Computations details
- DFT calculations
- VASP code
- PBE functional
- Climbing Image Nudge Elastic Band (CI-NEB) method

H$_2$ adsorption on TiC
Adsortion on (001) TiC surface: How it happens?

Experimental studies

Adsorption on C-Top Adsorption on Ti-Top
Kubas modes?

Models
- Supercell of (2x2)
- 64 atoms (32 C and 32 M)
- 2 fixed and 2 relaxed layers.
- 6 sites explored for H ads.
- 19 sites explored for H$_2$ ads.
(M-top, 1), (C-Top, 2), 4-fold hollow (4), 3-fold hollow formed by 2 metal and 1 Carbon atoms (MMC, 5), and 3-fold hollow formed by 2 Carbon and 1 metal atoms (CCM, 6).

Adsorption energy on different TMCs
$E_{ads} = E_{R/PMC} - (E_R - E_{TMC})$

Clean surface
H atom on vacuum

<table>
<thead>
<tr>
<th>E (eV)</th>
<th>TiC</th>
<th>VC</th>
<th>ZrC</th>
<th>NbC</th>
<th>δ-MoC</th>
<th>HfC</th>
<th>TaC</th>
</tr>
</thead>
<tbody>
<tr>
<td>H</td>
<td>-2.73</td>
<td>-2.13</td>
<td>-2.84</td>
<td>-2.01</td>
<td>-2.93</td>
<td>-2.77</td>
<td>-2.30</td>
</tr>
<tr>
<td>H$_2$</td>
<td>-0.46</td>
<td>0.01</td>
<td>-0.61</td>
<td>-0.07</td>
<td>-1.19</td>
<td>-0.93</td>
<td>-0.12</td>
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<tr>
<td>barrier</td>
<td>0.49</td>
<td>1.09</td>
<td>0.73</td>
<td>1.26</td>
<td>1.21</td>
<td>1.19</td>
<td>1.21</td>
</tr>
</tbody>
</table>

Most stable H adsorption site: C-top, except in TaC, Ta-Top. Most stable H$_2$ adsorption site: C-top on TiC, ZrC, δ-MoC, and HfC. M-top on VC, NbC, and TaC.

Reaction profile of H$_2$ dissociation

Conclusions
- H$_2$ dissociation occurs on (001) TiC surface.
- TiC barrier: 0.49 eV. The best candidate to produce H$_2$ dissociation.
- The order to cover the surface was found: First H atoms are adsorbed on C-Top, secondly H atoms are adsorbed on Ti-Top and, finally, H$_2$ molecules are physisorbed on Ti-Top.
- 3 different H sites are found: H adsorbed on C-Top and on Ti-Top, and H$_2$ molecules physisorbed on Ti-Top.
- Computational studies were done on other TMCs so to find candidates to perform experimental studies.
- Results show that H$_2$ dissociation is also thermodynamically favourable on TiC, ZrC, HfC, and δ-MoC.

References