Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Electronic Supplementary Information

A density functional theory study of hydrogen dissociation and diffusion at the perimeter sites of Au/TiO_2

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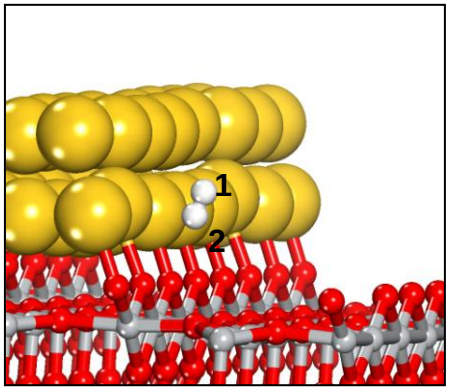
The optimized Au-H, O-H and H-H distances in all structures

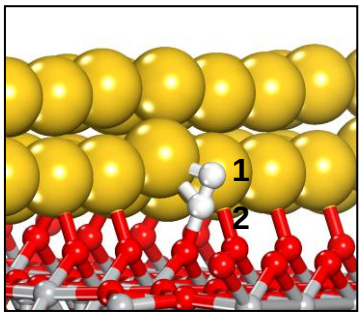


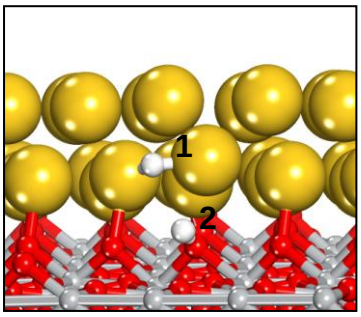
Adsorption state:

H_1-Au : 2.81 Å; H_1-O : 3.36 Å;

H_2-Au : 2.51 Å; H_1-O : 2.63 Å;

H_1-H_2 : 0.76 Å

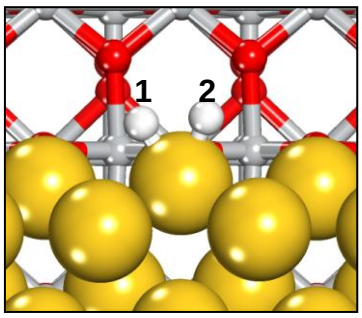


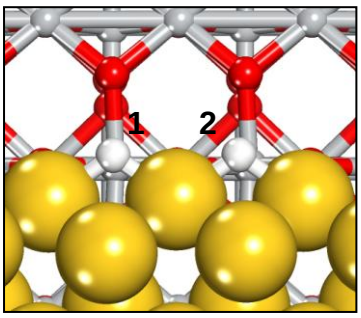


Heterolytic dissociation:

Transition state: H_1-Au : 1.81 Å; H_2-O : 1.43 Å; H_1-H_2 : 0.95 Å

Final state: H_1-Au : 1.81 Å, 1.77 Å; H_2-O : 0.97 Å; H_1-H_2 : 2.55 Å

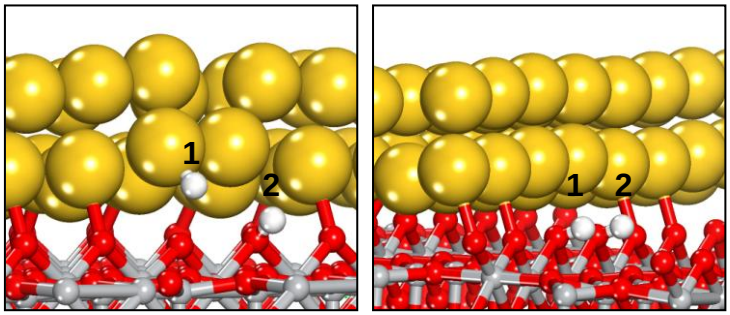




Homolytic dissociation:

Transition state: H_1-Au : 1.63 Å; H_2-Au : 1.62 Å; H_1-H_2 : 1.46 Å

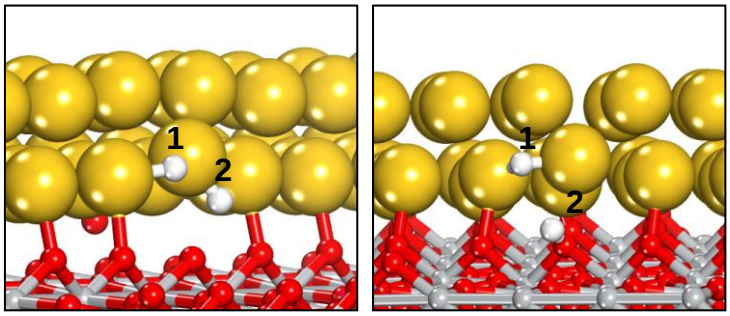
Final state: H_1-Au : 1.82 Å, 1.76 Å; H_2-Au : 1.82 Å, 1.76 Å; H_1-H_2 : 2.86 Å



Diffusion from heterolytic dissociation:

Transition state: H_1-Au : 1.60 Å; H_1-O : 1.80 Å; H_2-O : 0.97 Å; H_1-H_2 : 2.93 Å

Final state: H_1-Au : 2.77 Å; H_1-O : 0.97 Å; H_2-O : 0.97 Å; H_1-H_2 : 2.98 Å



Diffusion from homolytic dissociation:

Transition state: H_1-Au : 1.81 Å, 1.75 Å; H_2-Au : 1.60 Å; H_2-O : 1.91 Å; H_1-H_2 : 0.95 Å

Final state: H_1-Au : 1.81 Å, 1.77 Å; H_2-Au : 2.74 Å; H_2-O : 0.97 Å; H_1-H_2 : 2.55 Å