Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Material: Tetra-penta-deca-hexagonal-graphene (TPDH-graphene) hydrogenation patterns: dynamics and electronic structure

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Table S.1: Binding energies of the investigated configurations for adsorption. Beginning with the non-equivalent sites, H atoms are added to the most favorable structures taken as those with highest E_b. The sequence of sites indicates the order of adsorption.

Adsorbed Sites	Binding Energy (eV)
C1	3,35
C1'	3,35
C2	2,43
C3	2,34
C4	2,65
C5	3,35
C5'	3,35
C6	3,35
C6'	3,35
C7	3,35
C7'	3,35
C1-C2	3,04
C1-C3	2,70
C1-C4	2,78

Adsorbed Sites	Binding Energy (eV)
C1-C5	3,65
C1-C5’	2,88
C1-C6	2,91
C1-C6’	3,20
C1-C7	3,33
C1-C7’	3,75
C1-C7’-C5	3,65
C1-C7’-C5’	3,26
C1-C7’-C6	3,26
C1-C7’-C6’*	3,65
C1-C7’-C5-C6	3,50
C1-C7’-C5-C6'	4,00

Figure S.1: Hydrogen adsorption rates for T = 150 K.

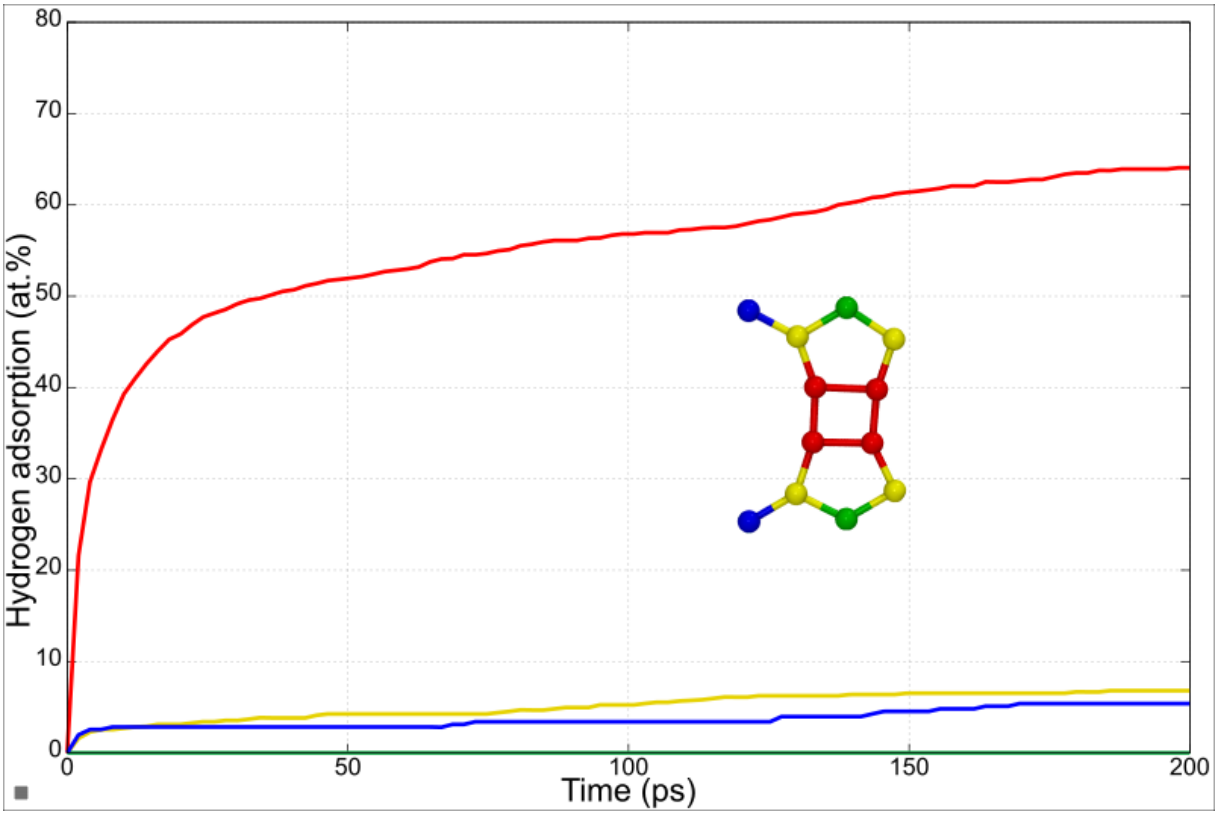

Figure S.2: Hydrogen Adsorption rates for T = 300 K.

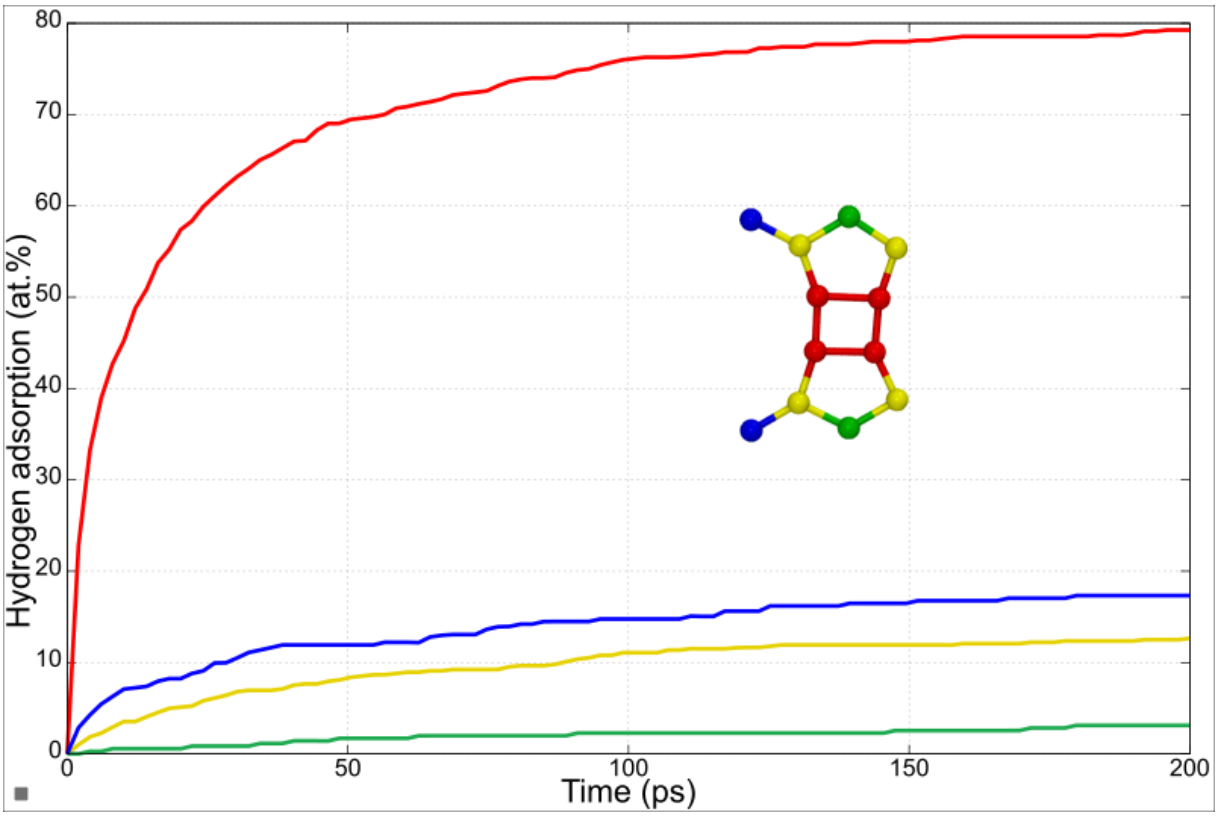

Figure S.3: Hydrogen adsorption rates for T = 500 K.

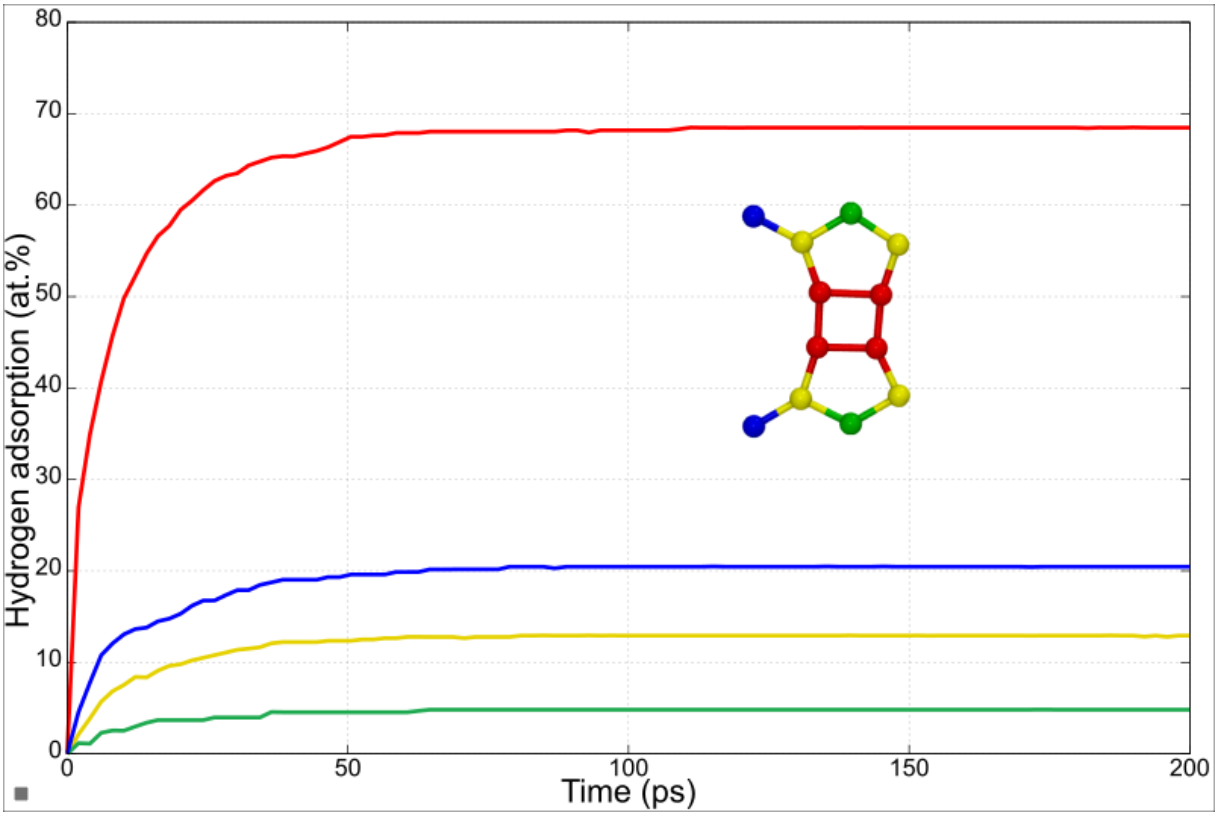

Figure S.4: Hydrogen adsorption rates for T = 800 K.