

Electronic Supplementary Information

The effect of the stacking fault on the diffusion of chemisorbed hydrogen atoms inside few-layered graphene

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Gyeonggi-do 463-400, Korea

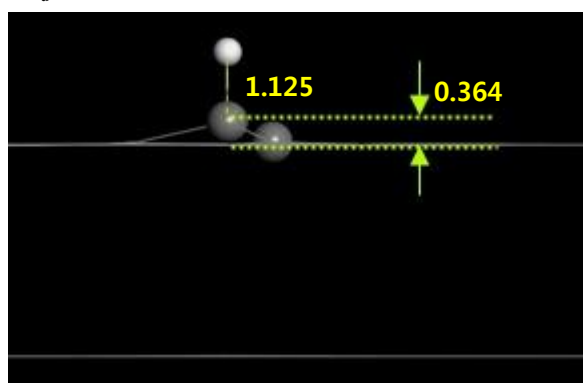
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Seongbuk-gu, Seoul 136-791, Korea

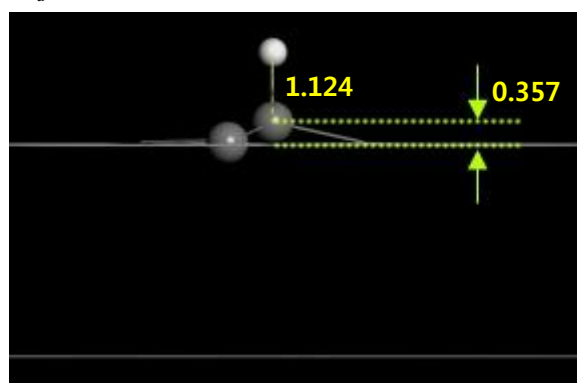
^dInterdisciplinary School of Green Energy and Low Dimensional Carbon Materials Center, Ulsan
National Institute of Science and Technology, UNIST-gil 50, Ulsan 689-798, Korea

a) BIL

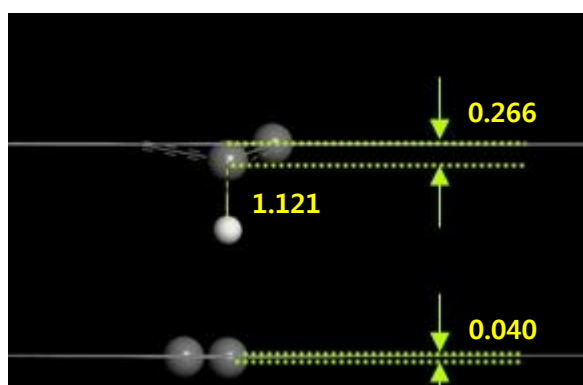
2A_u



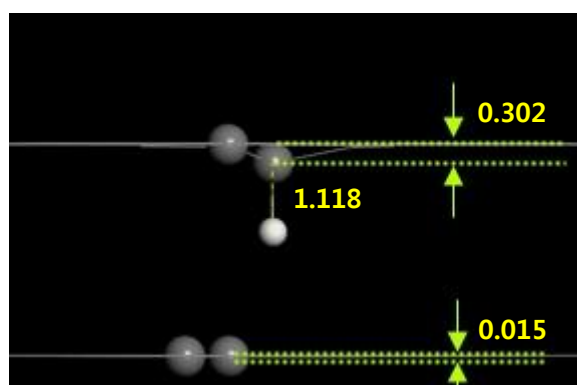
2B_u



2A_d

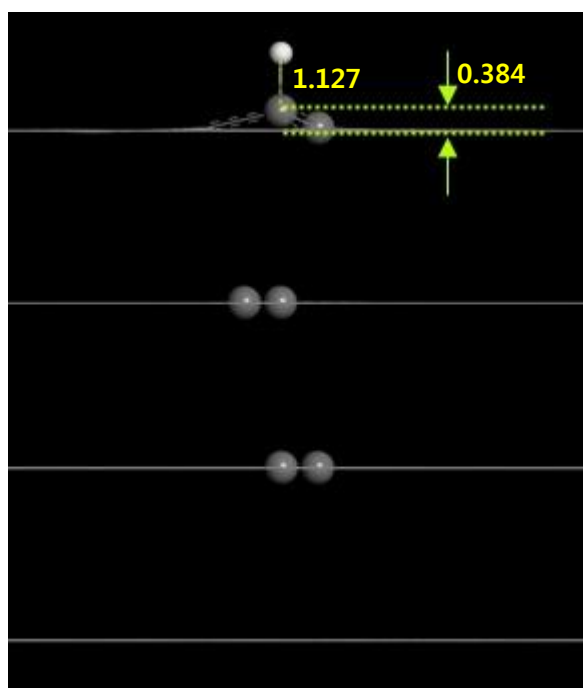


2B_d

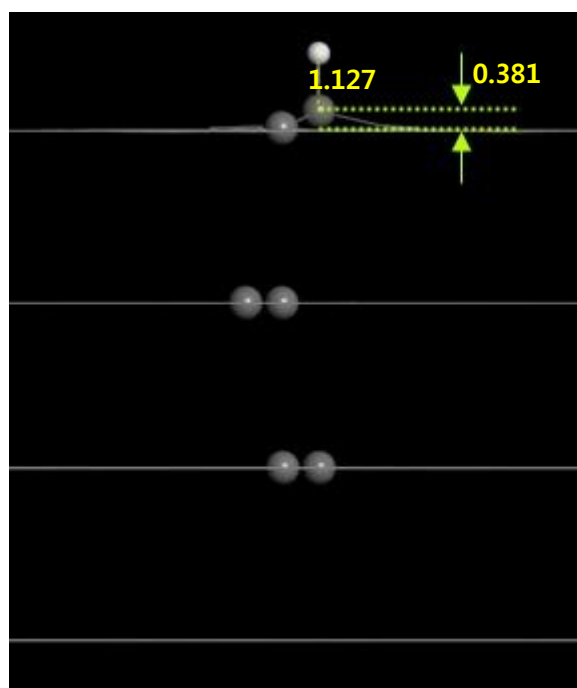


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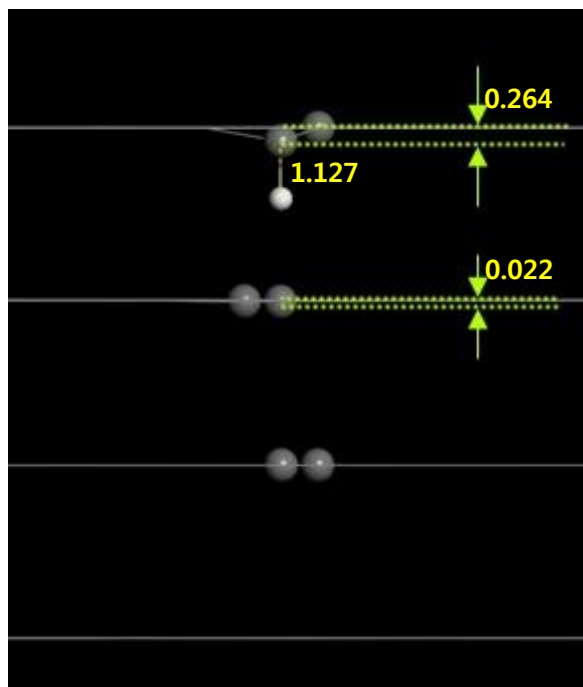
4A_u



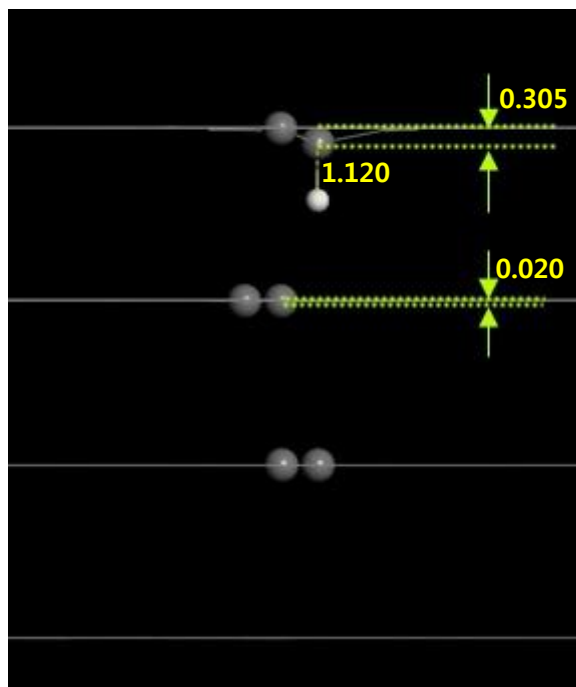
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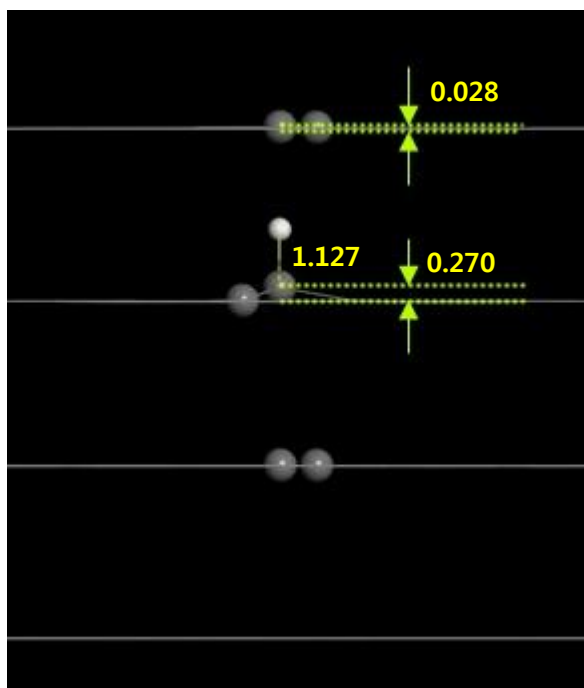
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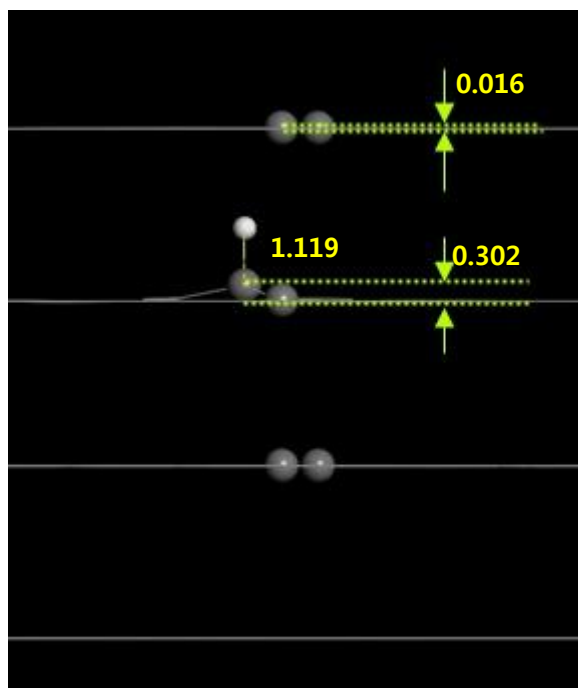
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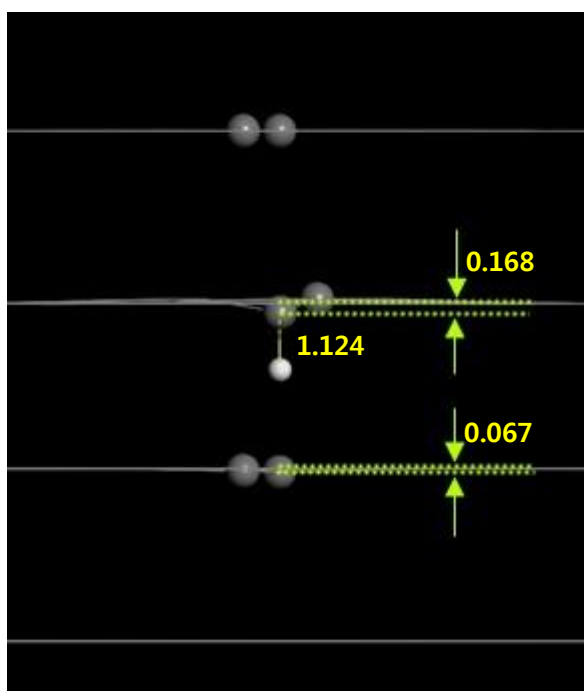
3A_u



3B_u



3A_d



3B_d

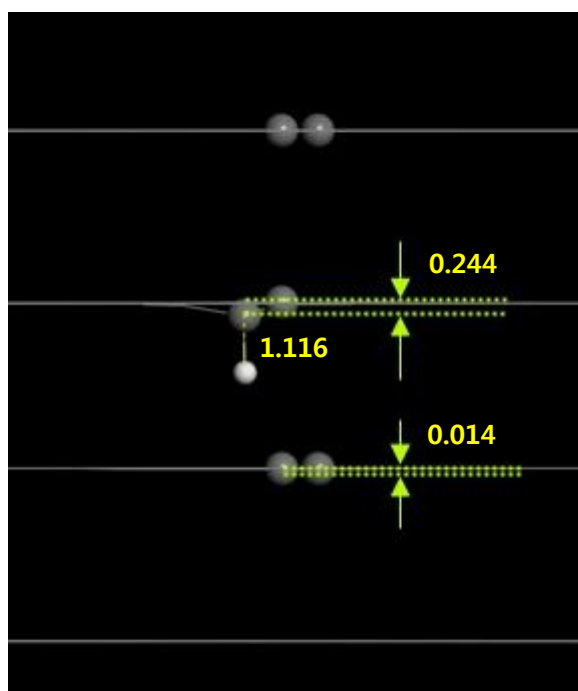
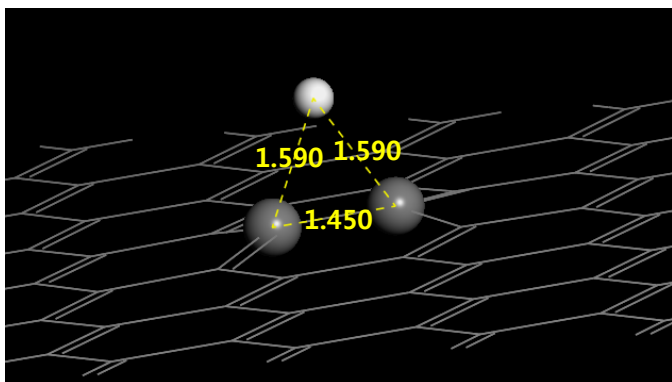


Fig. S1. The hydrogen binding structures in a) BIL, and b) TEL. The gray balls and lines are for graphene sheets and the white ball is the hydrogen atom. The unit of length is the angstrom.

a) MNL

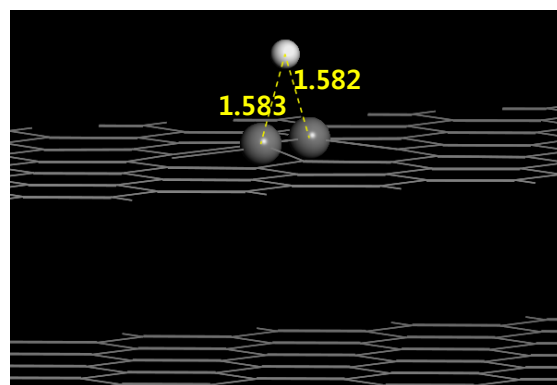
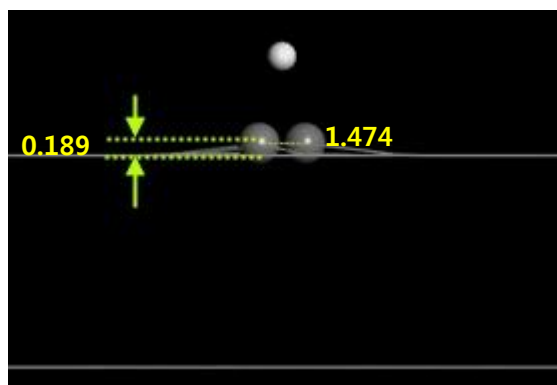


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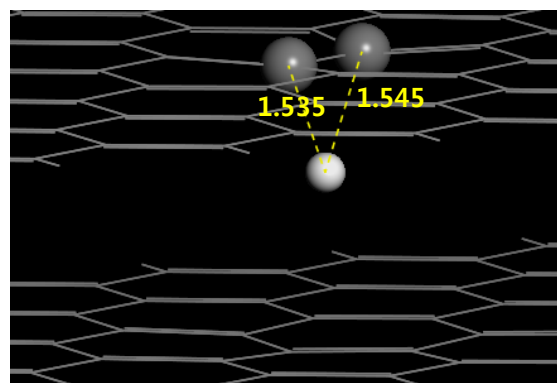
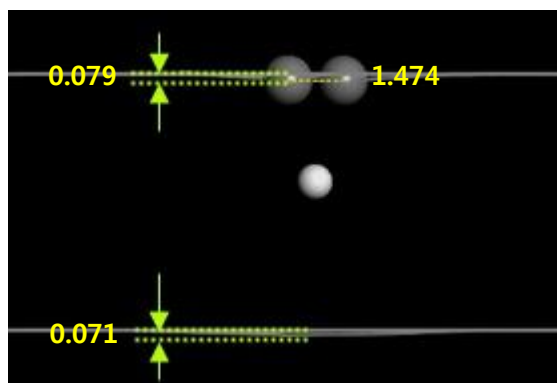
C-C distance

C-H distances

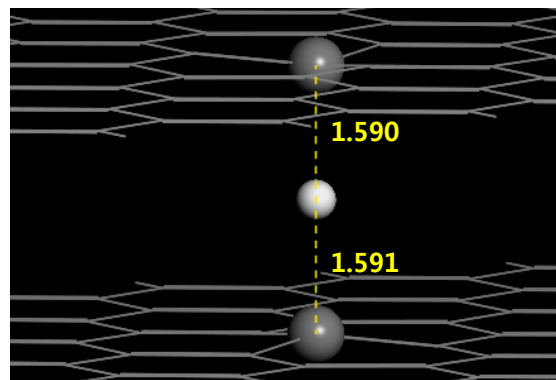
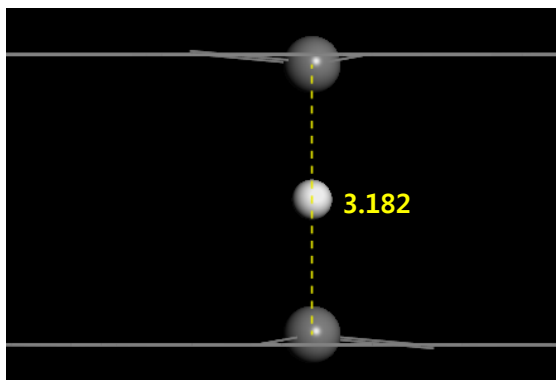
$2A_u \rightarrow 2B_u$



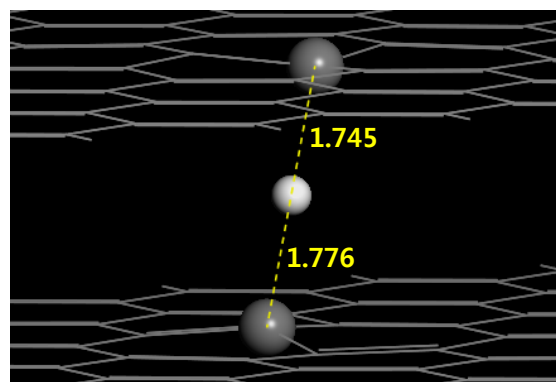
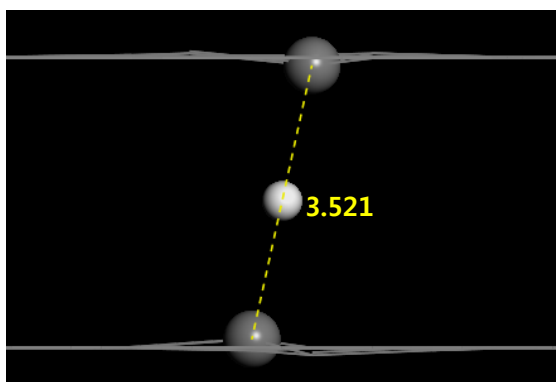
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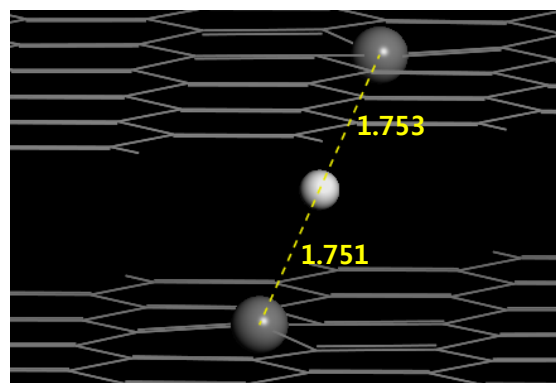
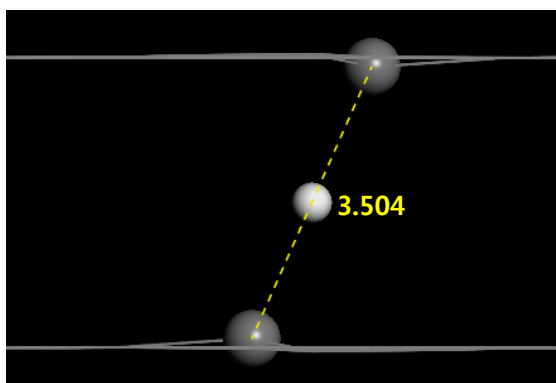
$2A_d \rightarrow 1A_u$



$2A_d \rightarrow 1B_u$



$2B_d \rightarrow 1B_u$

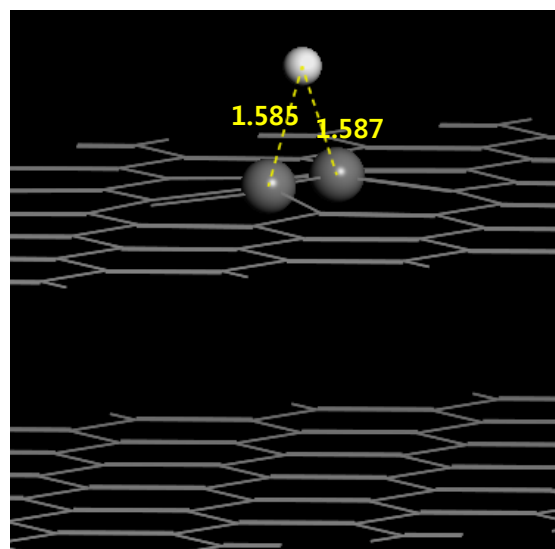
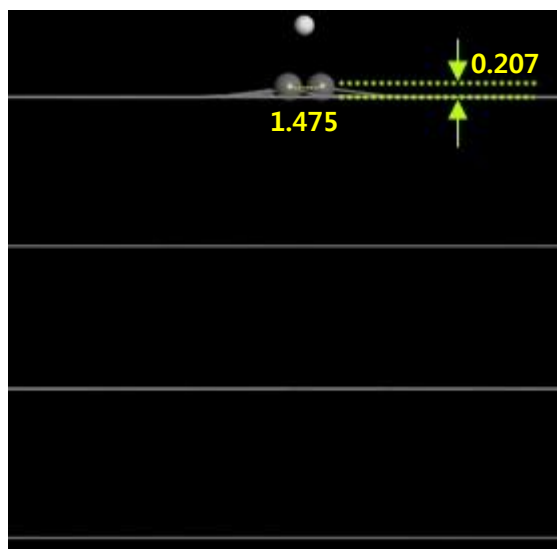


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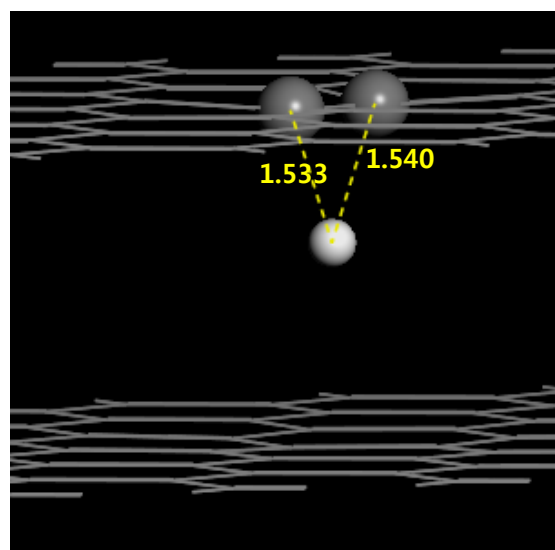
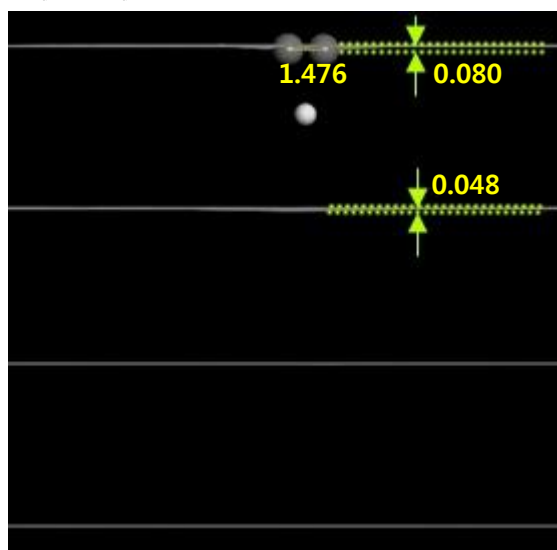
C-C distance

C-H distances

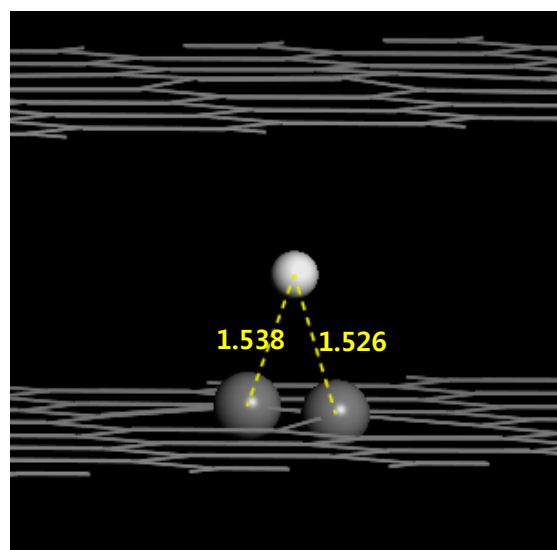
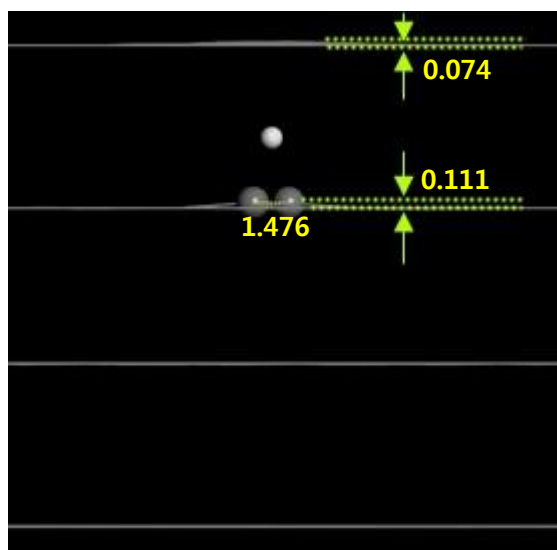
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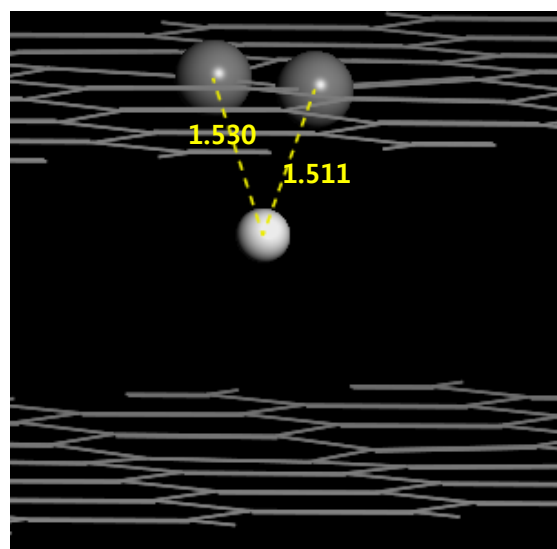
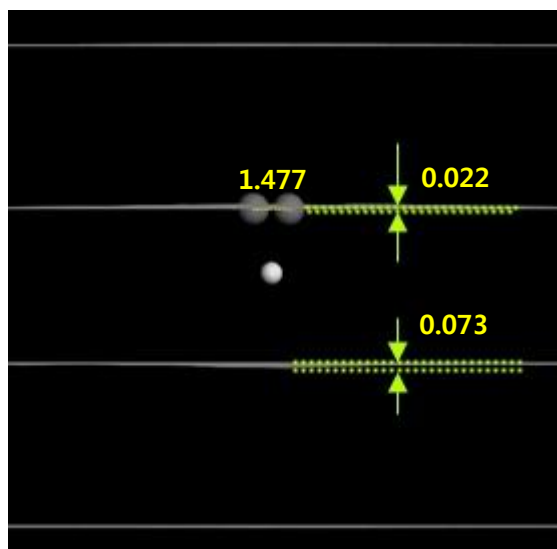
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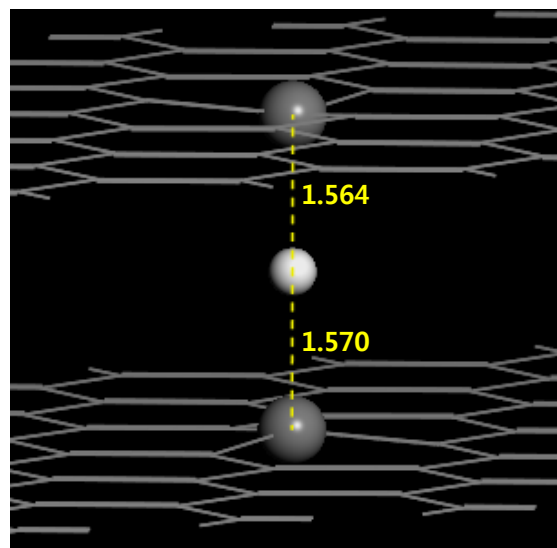
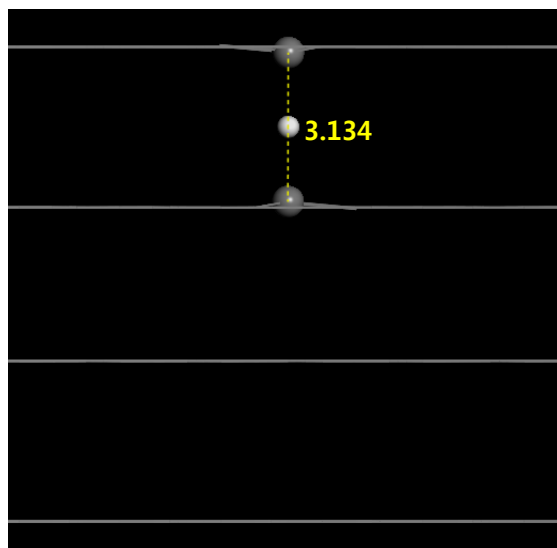
$3A_u \rightarrow 3B_u$



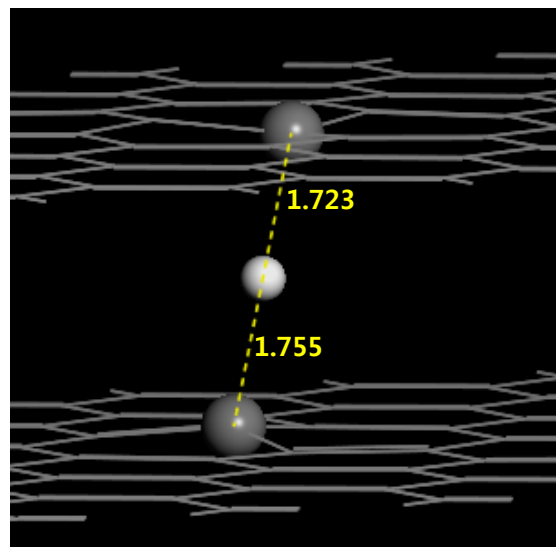
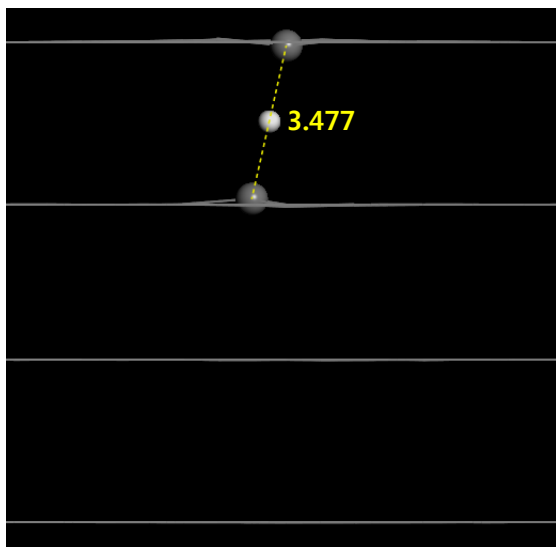
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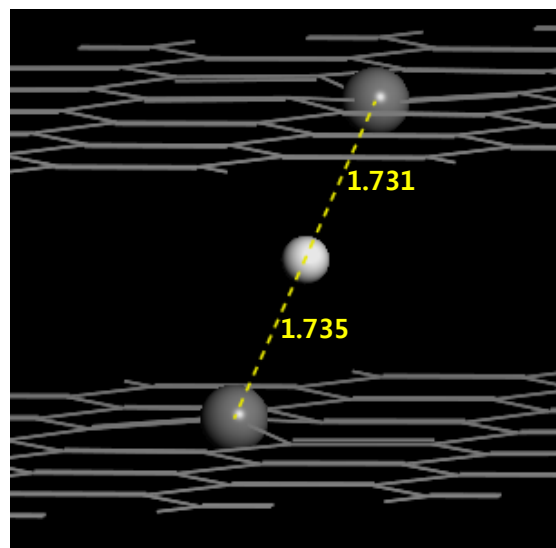
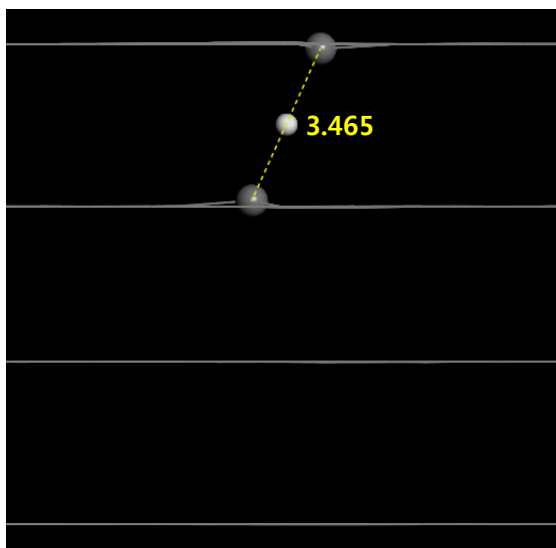
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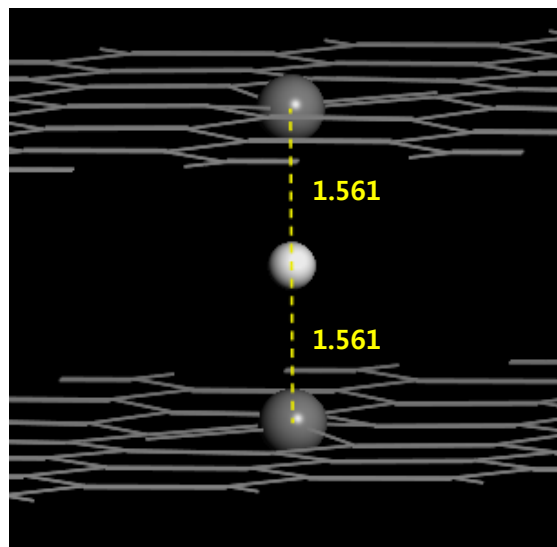
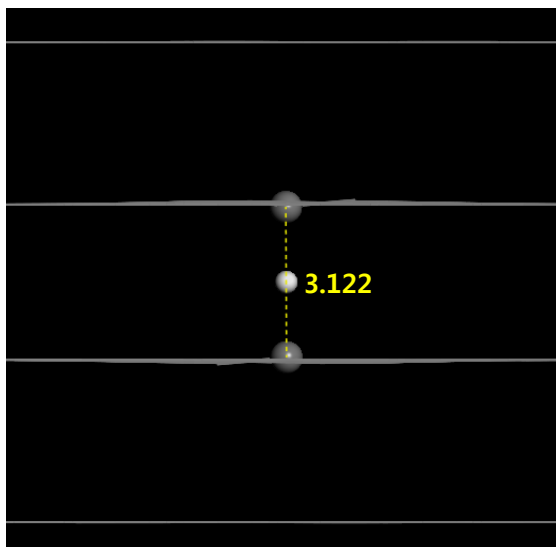
$4A_d \rightarrow 3B_u$



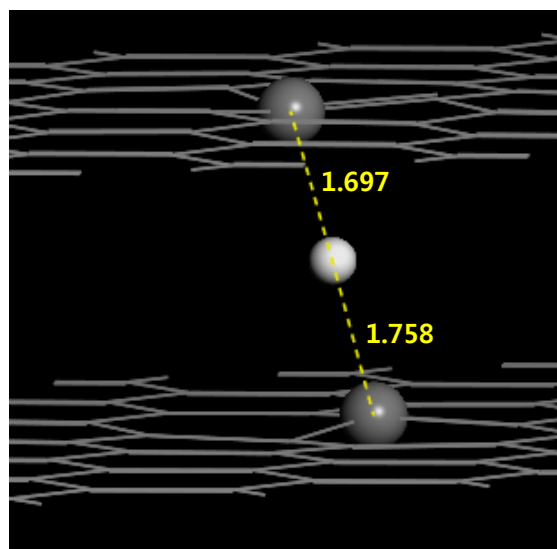
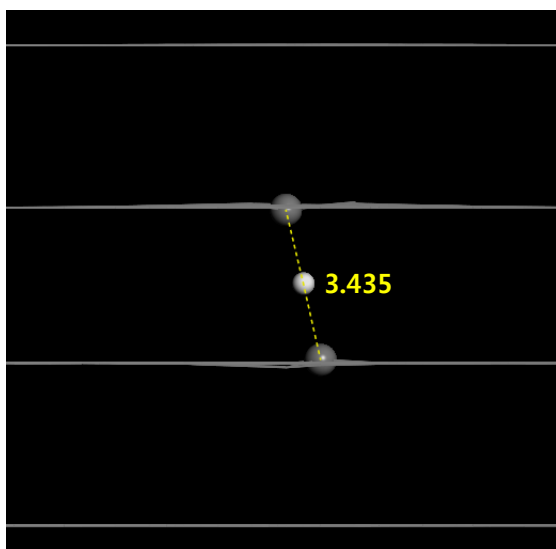
$4B_d \rightarrow 3B_u$



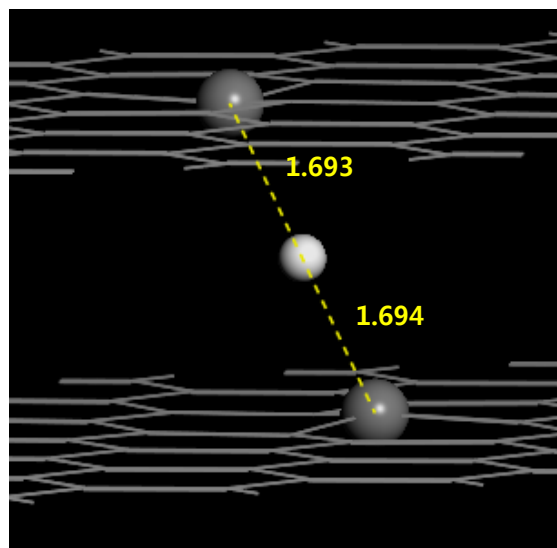
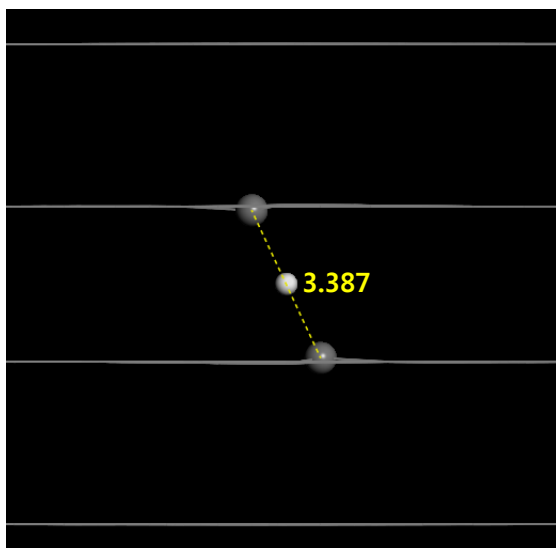
$3A_d \rightarrow 2A_u$



$3A_d \rightarrow 2B_u$



$3B_d \rightarrow 2B_u$

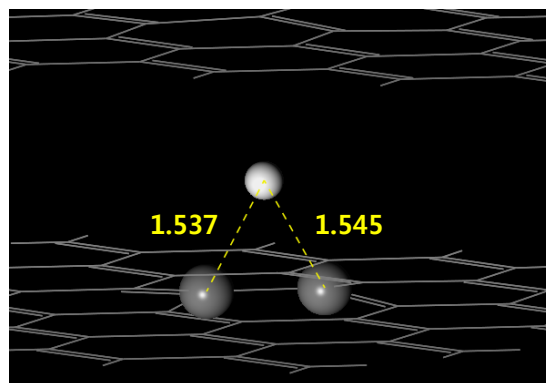
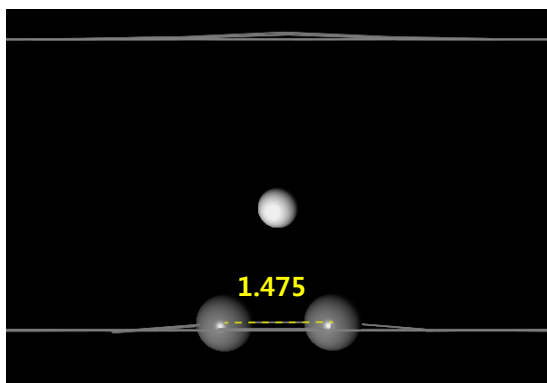


d) ZIG

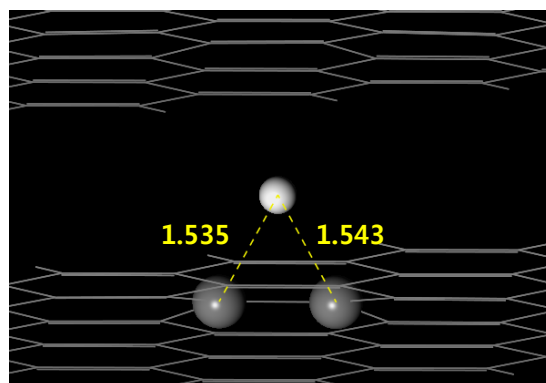
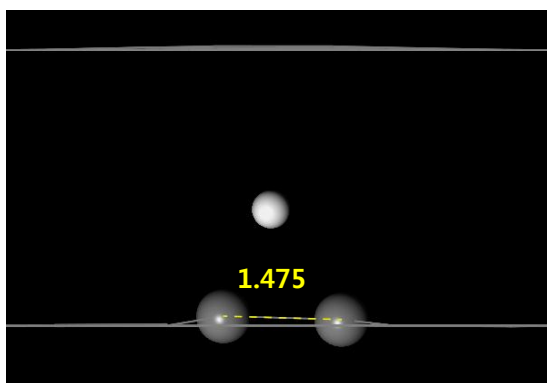
C-C distance

C-H distances

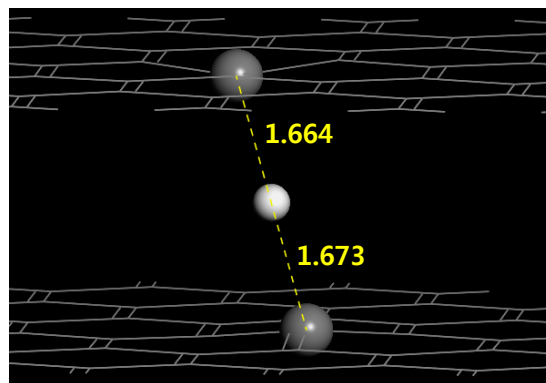
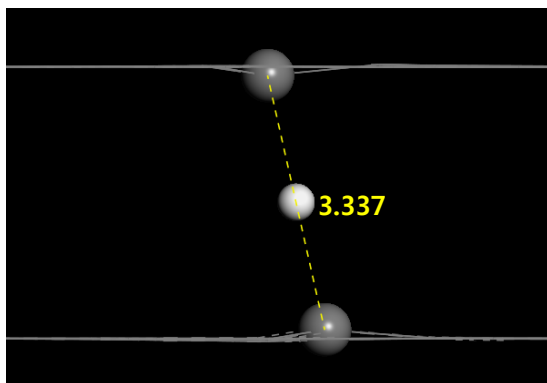
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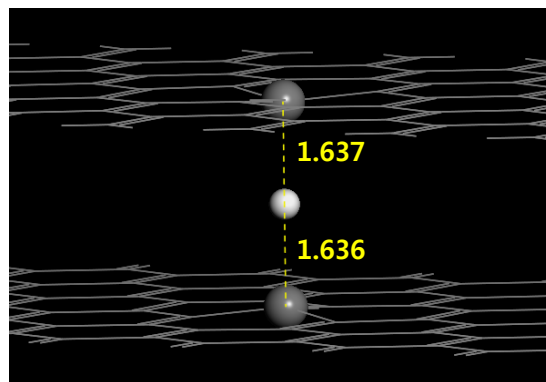
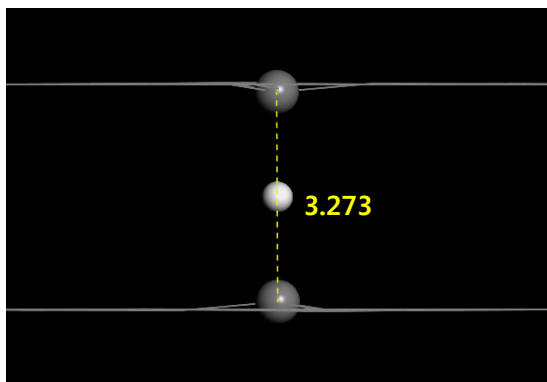
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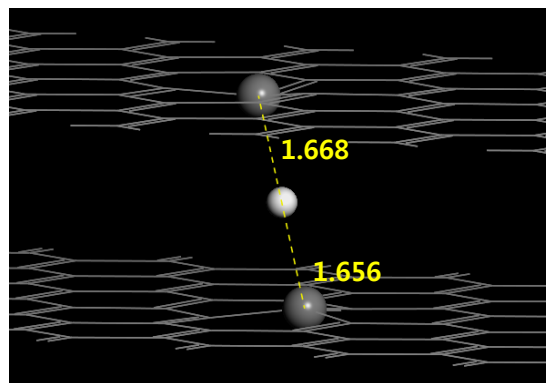
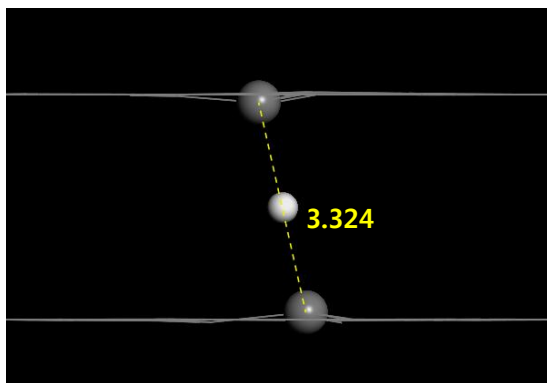
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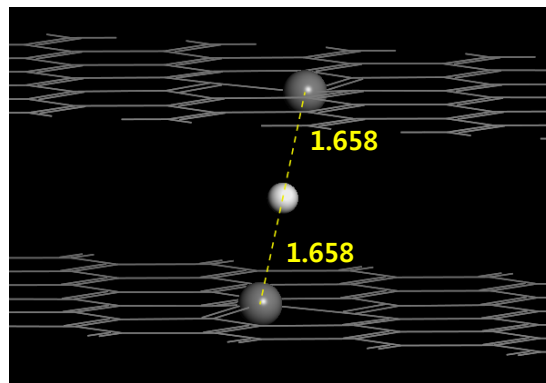
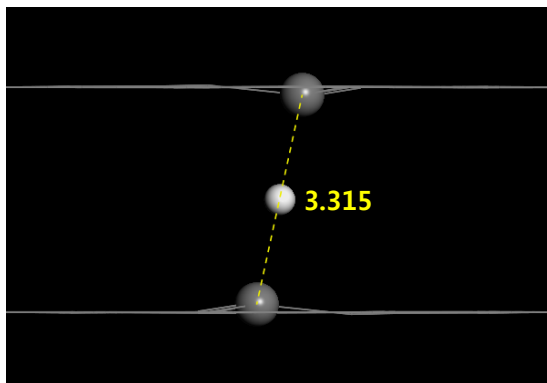
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5



6

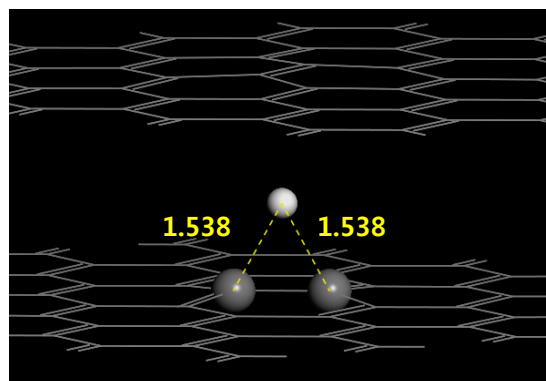
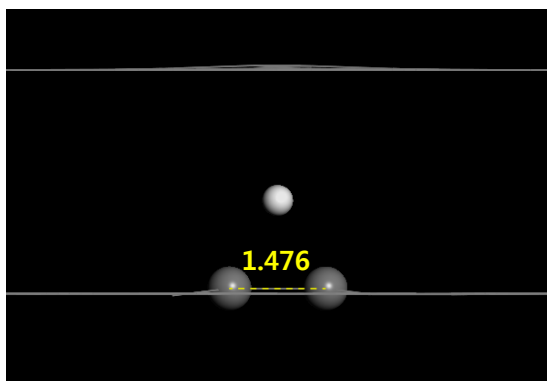


e) ARM

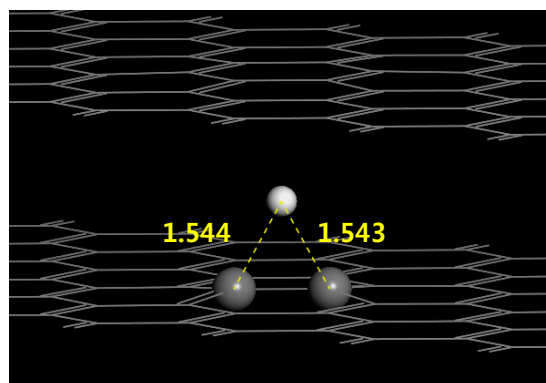
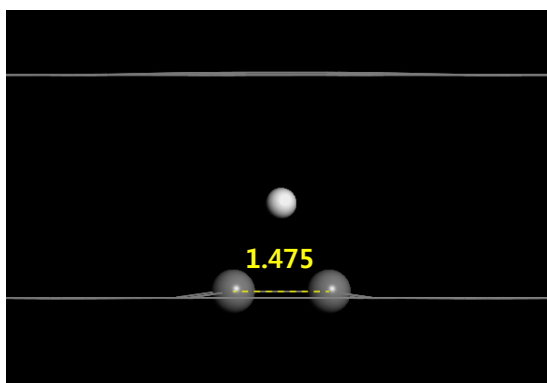
C-C distance

C-H distances

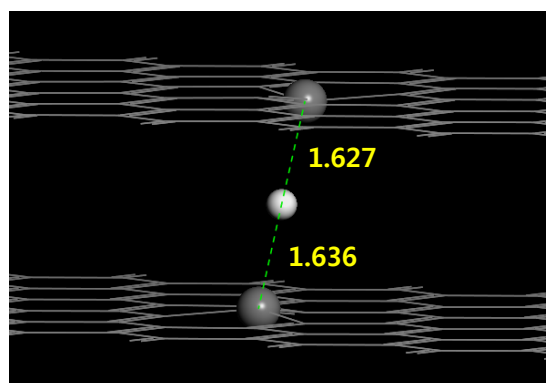
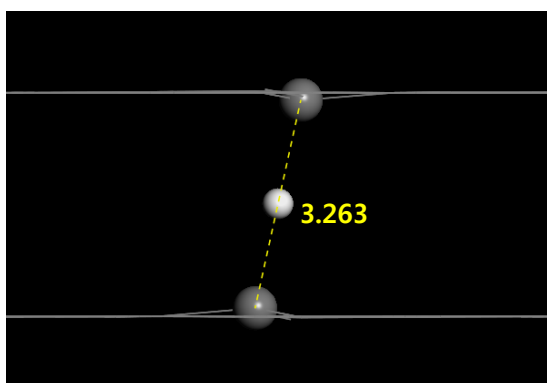
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2



3



4

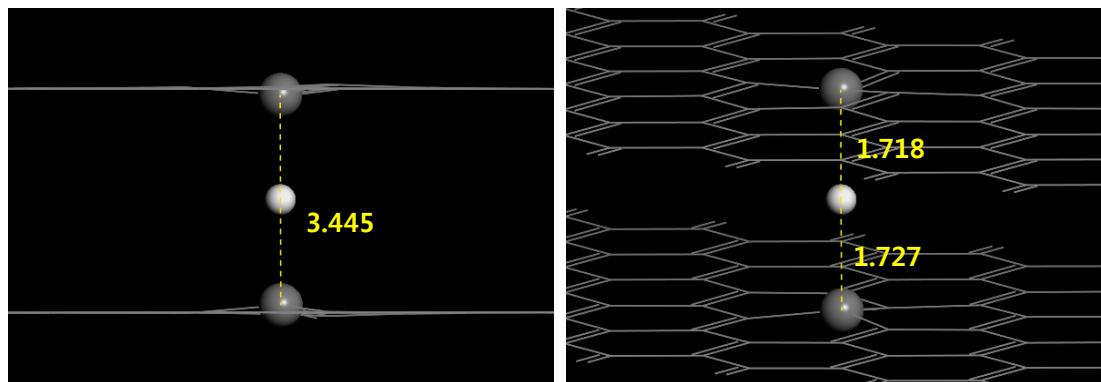


Fig. S2. The transition state structures. The gray balls and lines are for graphene sheets and the white ball is the hydrogen atom. The unit of length is the angstrom.

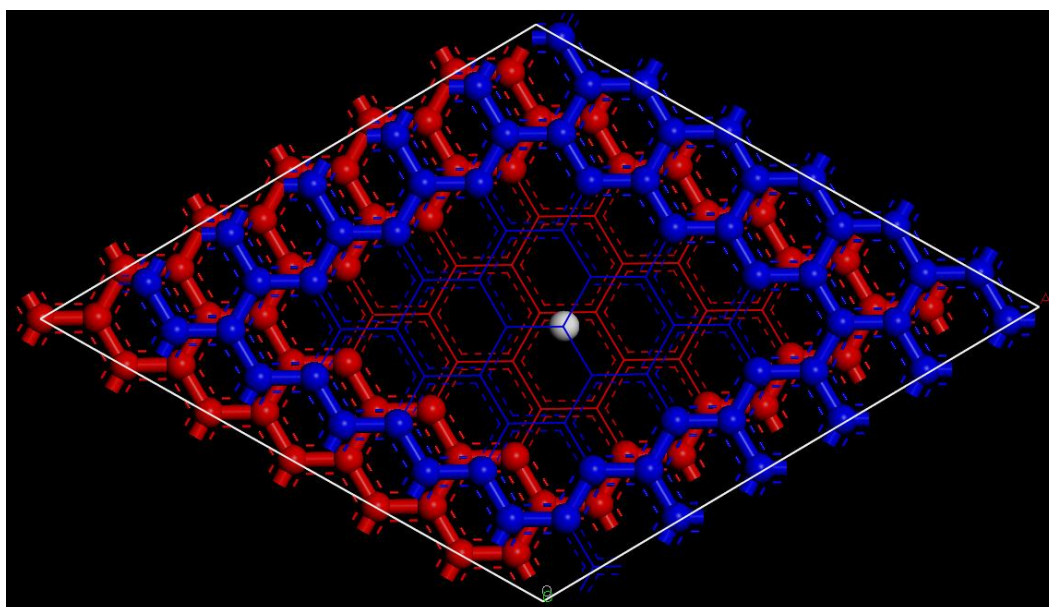


Fig. S3. The ball-and-stick model represents the fixed carbon atoms. The blue carbons are in the upper layer and the red ones are in the lower layer.