H_2S adsorption on NH-decorated graphene: A first principles study

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Highlights

- Adsorption and dissociation of H_2S molecule on NH-doped graphene were studied.
- We predicted that the adsorption of H_2S was enhanced by the nitene radicals (NH)
- We showed that there is partial dissociation at a weight percent of 3.76 wt% of NH radical.
- We also observed a complete dissociation of H_2S molecule at 7.25 wt% NH radical.
- The H-transfer of the second H atom of H_2S molecule at 3.76 wt% was energetic unfavorable.