## Li-decorated carbon ene-yne as a potential high-capacity hydrogen storage medium

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Figure S1: The optimized atomic structures of one Li decorated CEY. The yellow and blue balls represent the C and Li atoms, respectively.



Figure S2: Density of states of pristine CEY and Li-decorated CEY based on HSE06.



Figure S3: Top and side views of the snapshots from ab initio molecular dynamics simulation for  $H_2$  adsorption on Li-decorated CEY at the temperature of 350 K.