**Supplementary Information**

**Electrocatalytic Hydrogen Evolution on the** **noble metal-free MoS2/carbon nanotube heterostructure: A theoretical study**

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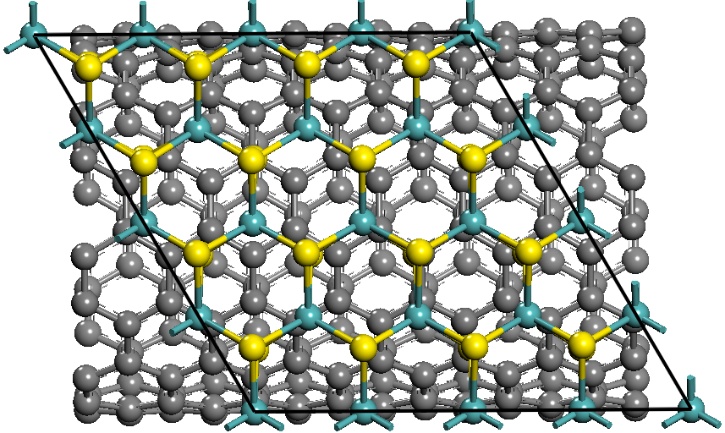
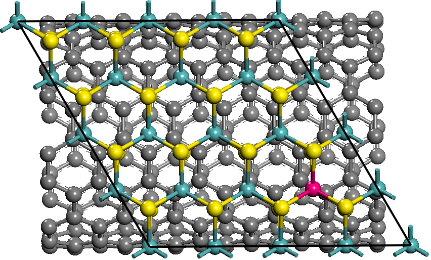
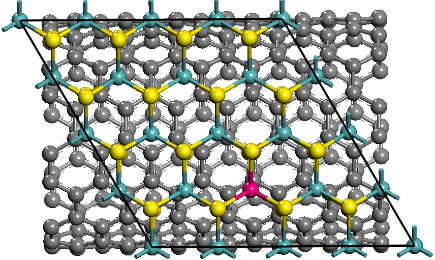
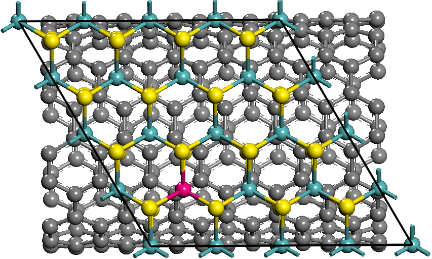
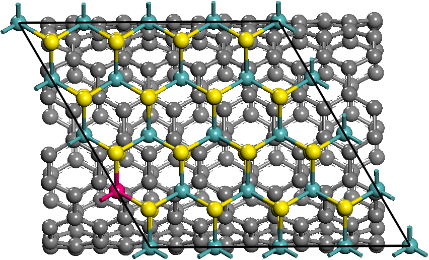
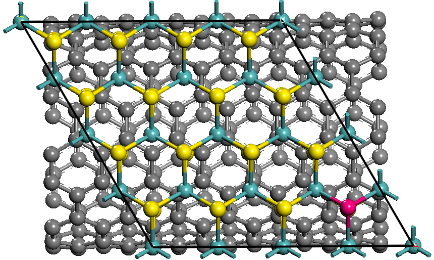
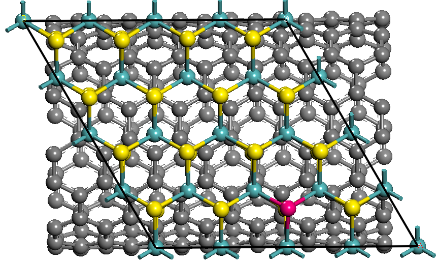
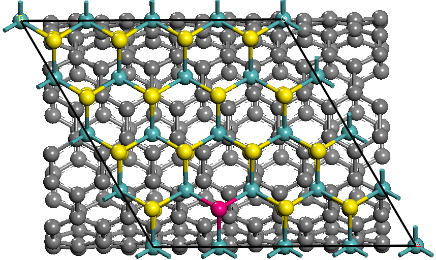
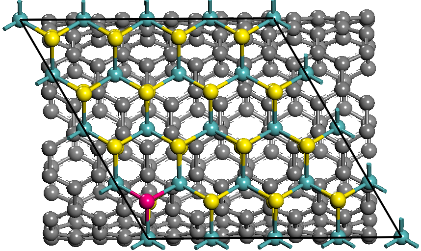
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**S1**

**S2**

**S3**

**S4**

**M1**

**M2**

**M3**

**M4**

**Figure S1.** Schematic view of the atomic charge on the MoS2/CNT heterostructure for different positions of sulfur (S1-S4) and molybdenum (M1-M4) atoms. BIOVIA, Dassault Systèmes, Materials Studio, version 7. https://bit.ly/38lRRQR

**Table S1**. Atomic charge values on the MoS2/CNT heterostructure

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Site location | S1 | S2 | S3 | S4 | M1 | M2 | M3 | M4 |
| Charge (a.u.) | -0.190 | -0.142 | -0.140 | -0.191 | 0.221 | 0.229 | 0.229 | 0.220 |