Electronic Supplementary Material (ESI) for Journal of Materials Chemistry A.

Molybdenum Sulfide Clusters Immobilized on Defective Graphene: A Stable Catalyst for Hydrogen Evolution Reaction

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Supporting Information

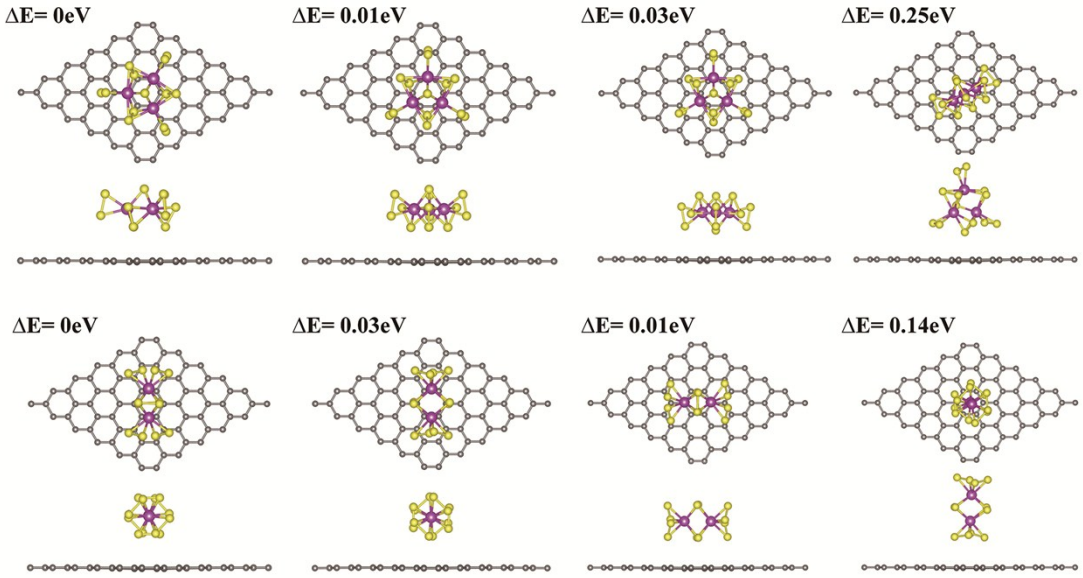

Fig. S1 Relaxed adsorption structures with energy difference for different configurations of the Mo3 and Mo2 on defect-free graphene. The total energy of the lowest energy configuration is used as the reference.

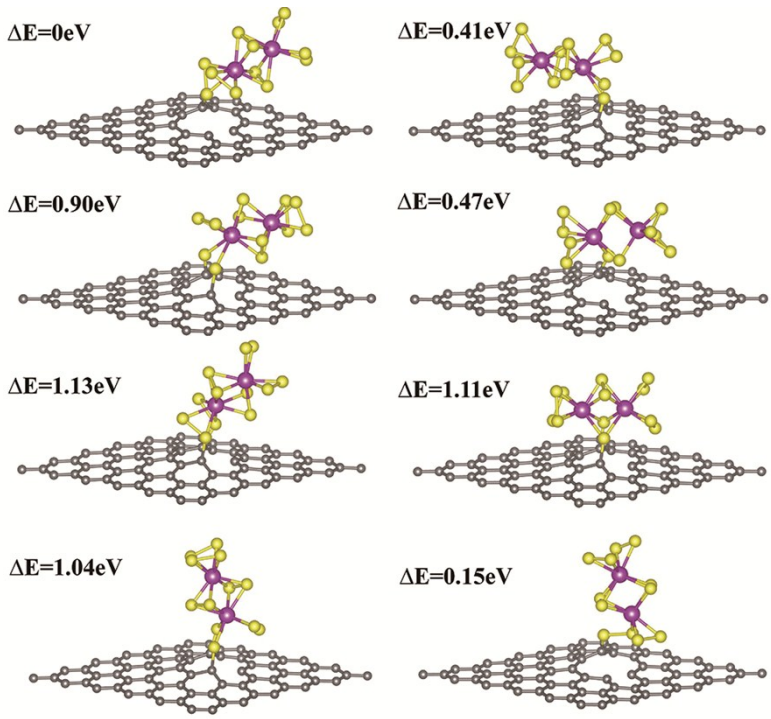

Fig. S2 Relaxed adsorption structures with energy difference for different configurations of the Mo2 on mono-vacancy graphene. The total energy of the lowest energy configuration is used as the reference.

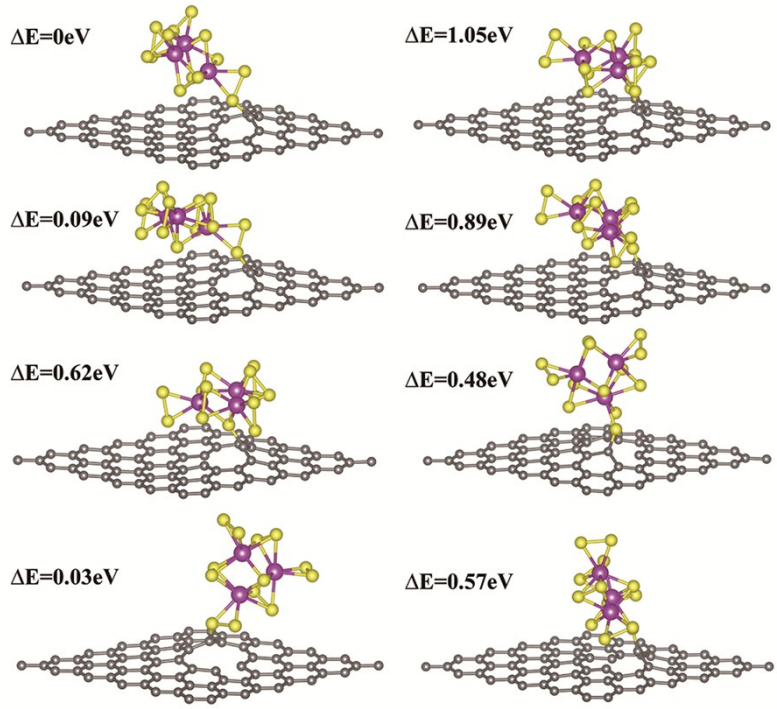

Fig. S3 Relaxed adsorption structures with energy difference for different configurations of the Mo3 on mono-vacancy graphene. The total energy of the lowest energy configuration is used as the reference.

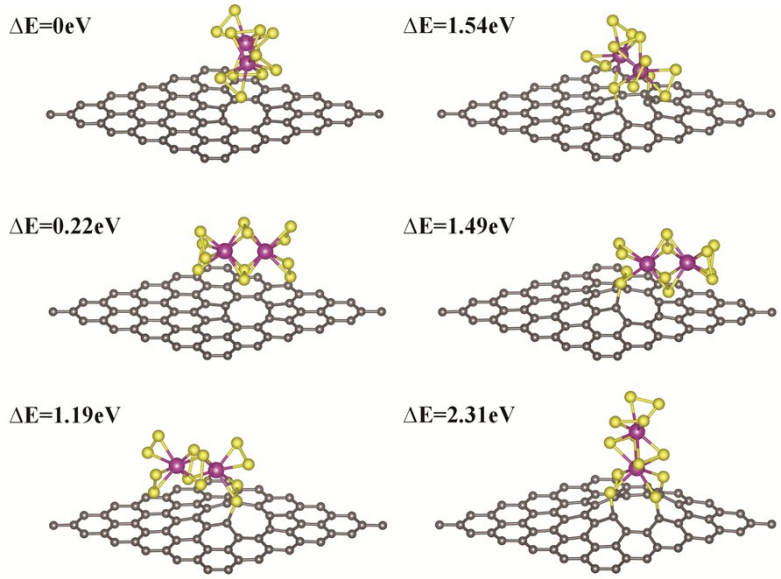

Fig. S4 Relaxed adsorption structures with energy difference for different configurations of the Mo2 on di-vacancy graphene. The total energy of the lowest energy configuration is used as the reference. The di-vacancy tends to form two pentagons and one octagon [V_2(5-8-5) defect] rather than forming S-C bonds with Mo2.

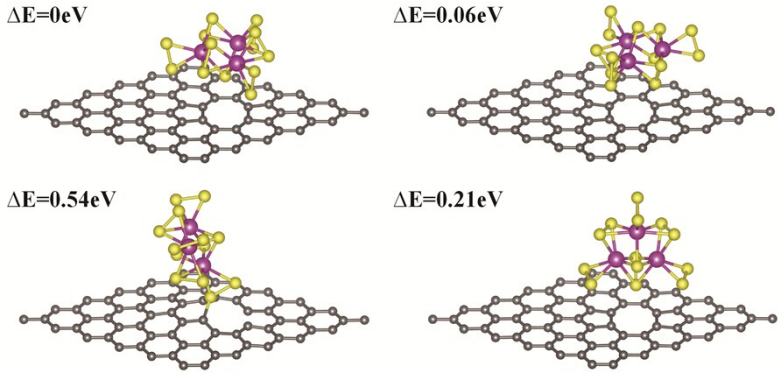

Fig. S5 Relaxed adsorption structures with energy difference for different configurations of the Mo3 on di-vacancy graphene. The total energy of the lowest energy configuration is used as the reference. The di-vacancy tends to form two pentagons and one octagon [V2(5-8-5) defect] rather than forming S-C bonds with Mo3.

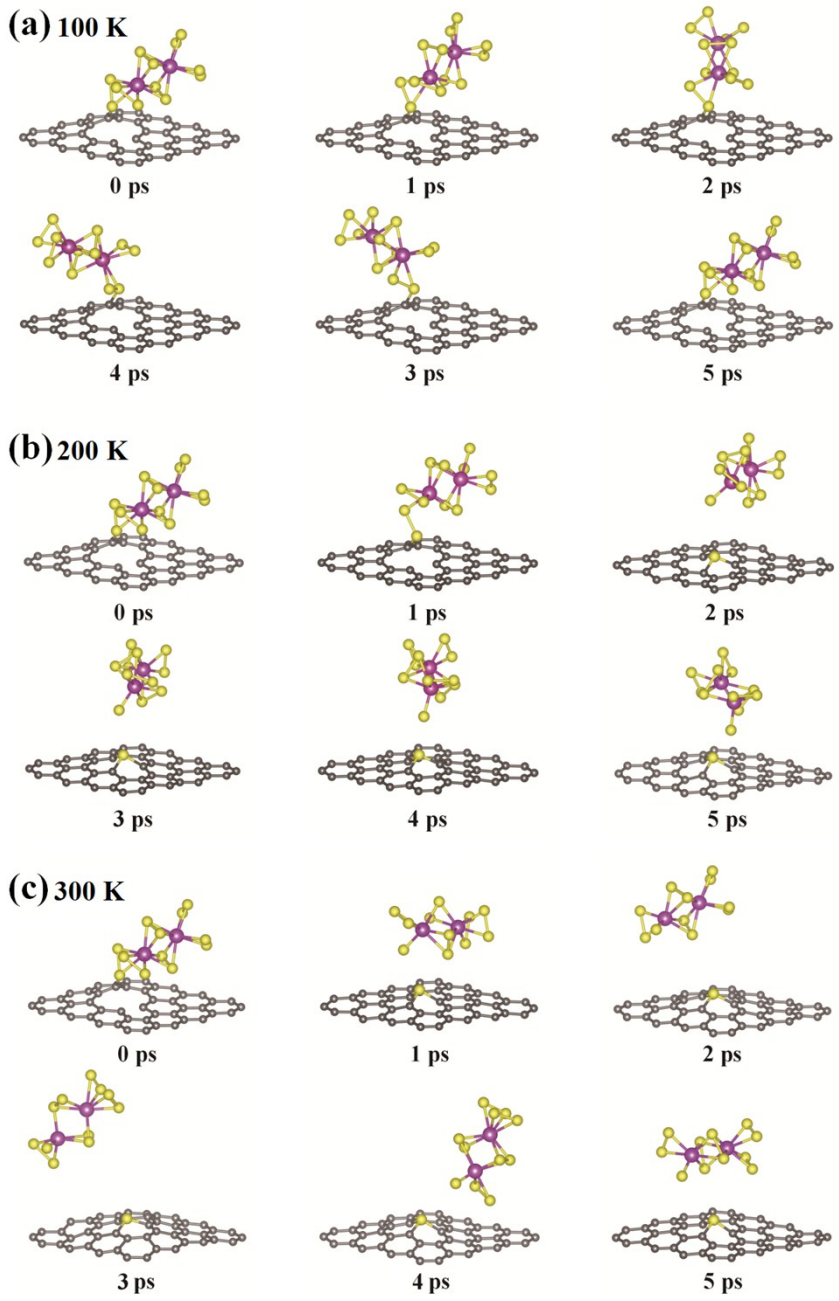

Fig. S6 Ab initio molecular dynamics simulations of structure evolution of the most stable chemisorption configurations of Mo2@graphene at (a)100K, (b)200K and (c)300K in 5 picoseconds.

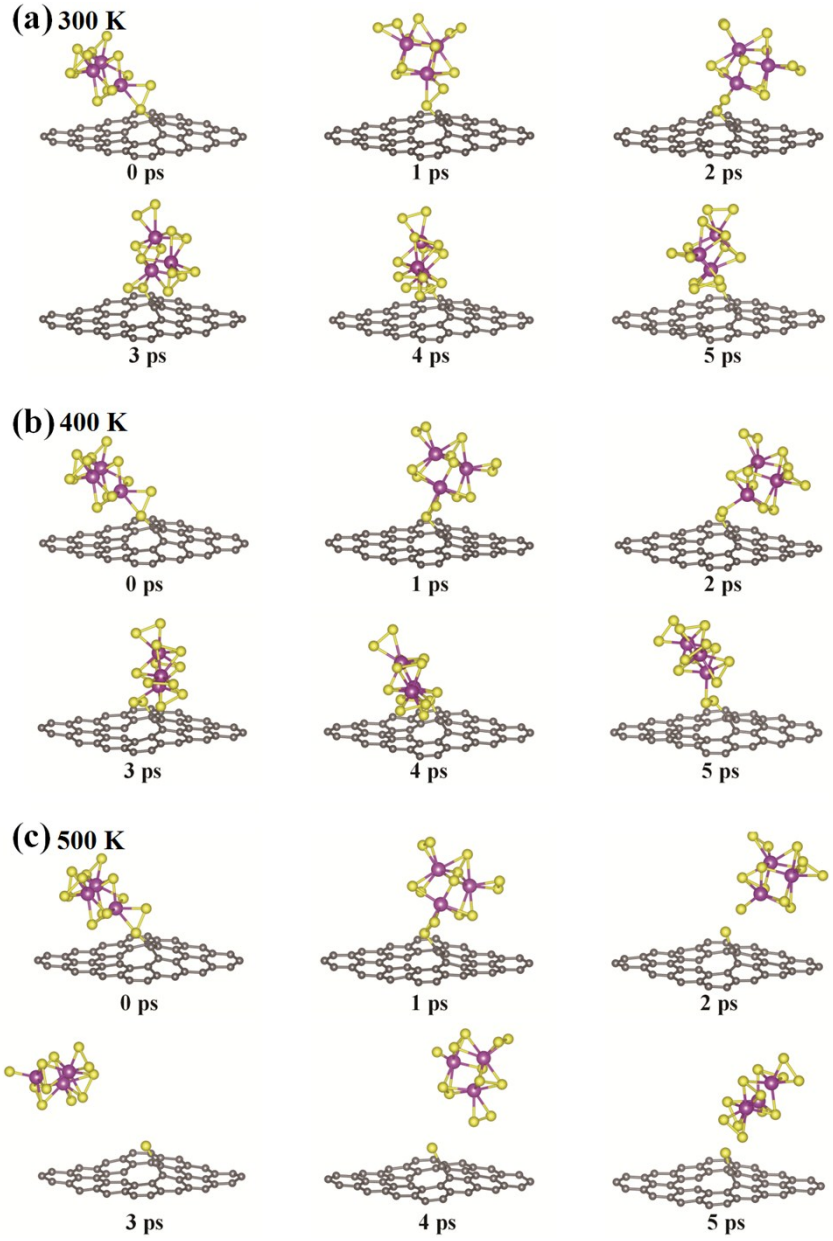

Fig. S7 Ab initio molecular dynamics simulations of structure evolution of the most stable chemisorption configurations of Mo3@graphene at (a)100K, (b)200K and (c)300K in 5 picoseconds.

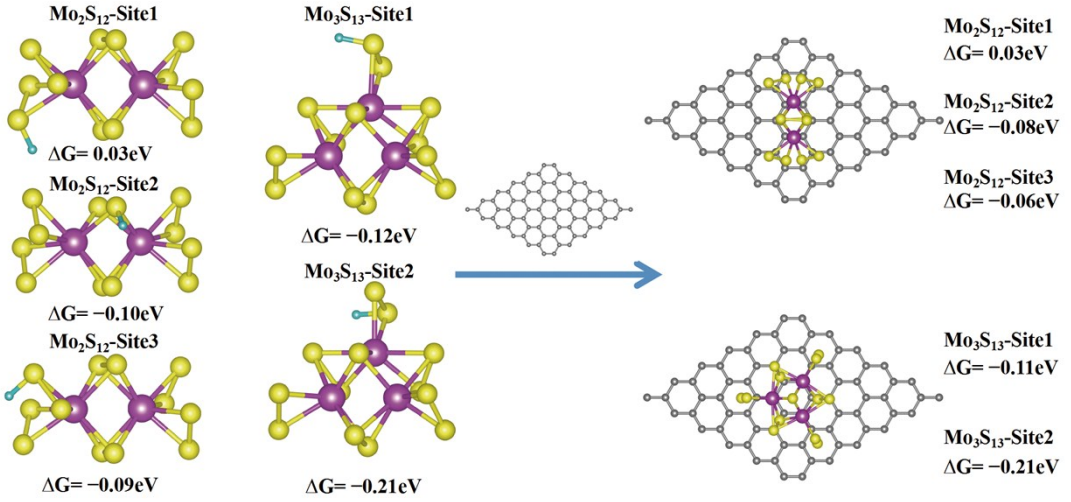

Fig. S8 Favorable H adsorption configurations on Mo2 and Mo3 and ΔG of Mo2 and Mo3 on graphene support.

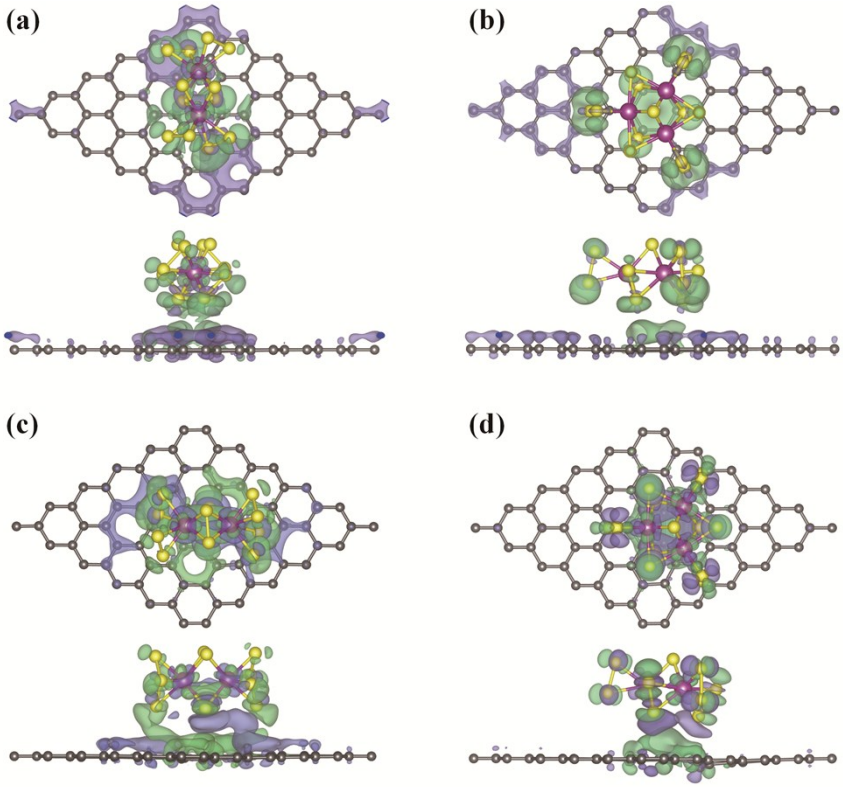

Fig. S9 Charge density difference of (a) Mo2 and (b) Mo3 on defect-free graphene, (c) Mo2 and (d) Mo3 on graphene with mono-vacancy. Depletion and accumulation spaces are revealed in green and blue, respectively.

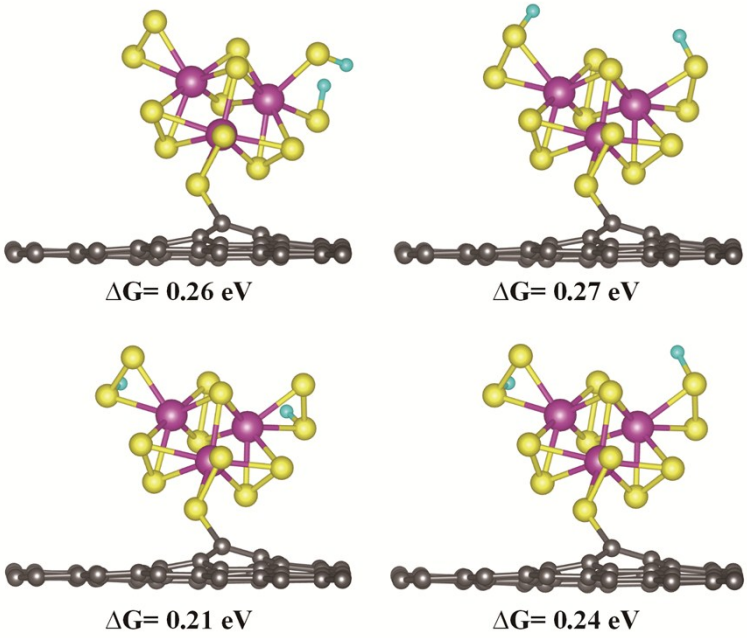

Fig. S10 Four most favorable 2H adsorption configurations on Mo3@Graphene. Their associated ΔG values are listed below each structure.