Supporting Information

Single-Atom Catalysts for Improved Cathode Performance in Na-S batteries: A Density Functional Theory (DFT) study

Rahul Jayan, Md Mahbubul Islam*

Department of Mechanical Engineering, 5050 Anthony Wayne Dr. Detroit, MI – 48202, USA

*Corresponding Author: gy5553@wayne.edu

Contents:

Number of pages: S12

Number of figures: 13

Number of tables: 0

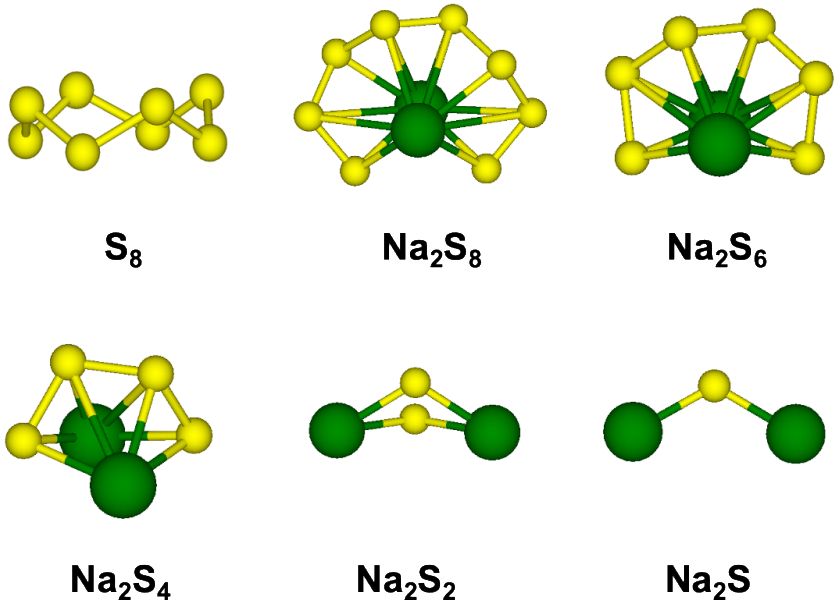

Figure S1. The optimized geometric structures of S_8 and NaPSs, Color codes: Yellow: Sulfur and Green: Sodium

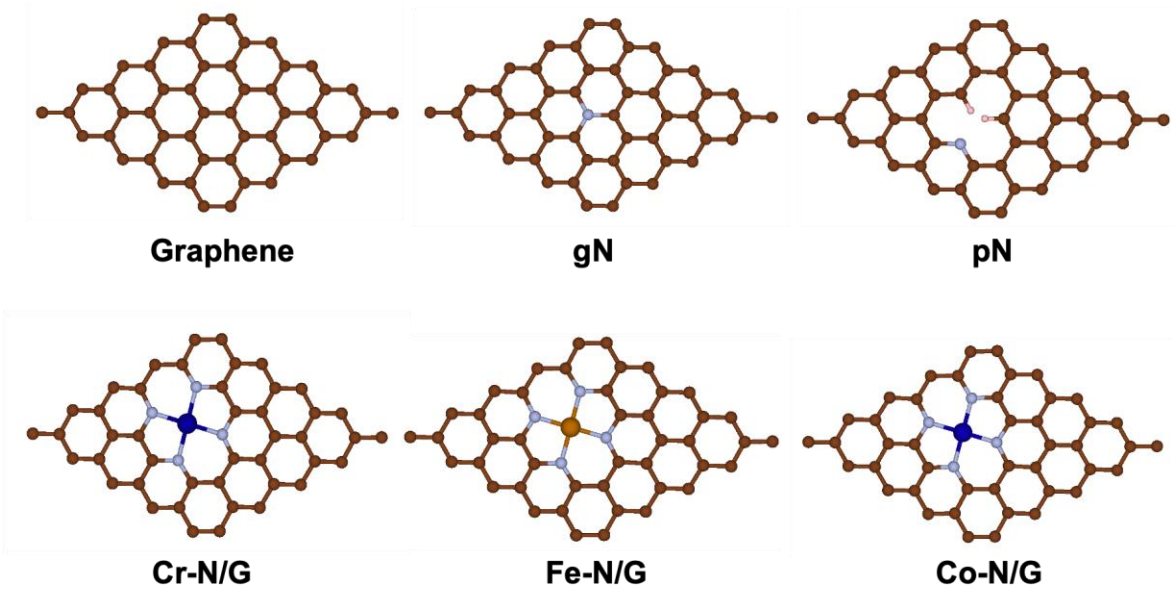

Figure S2. The top views of the most stable geometric structures of pristine and doped graphene substrates

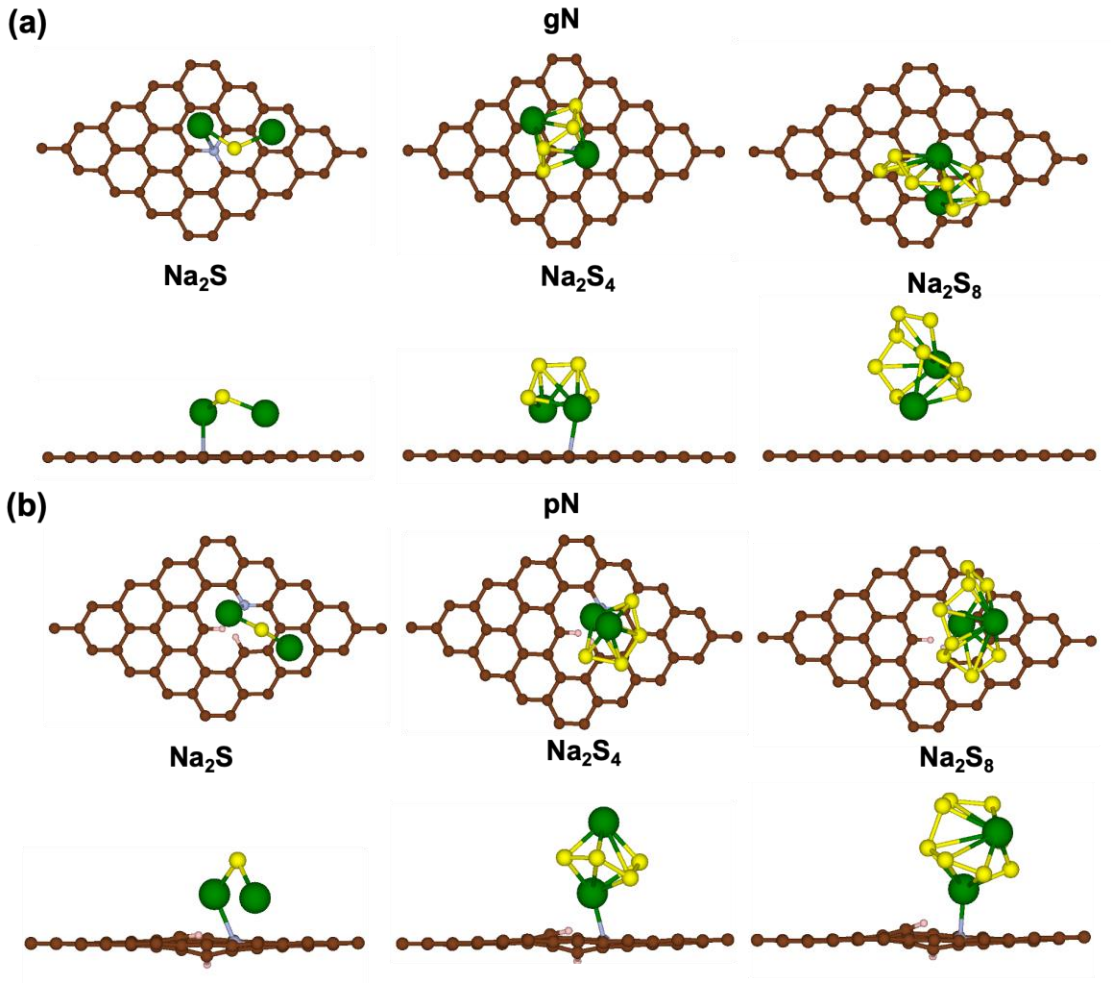

Figure S3. The top and side views of most stable geometric configurations of Na_2S_n adsorbed (a) gN and (b) pN structures.

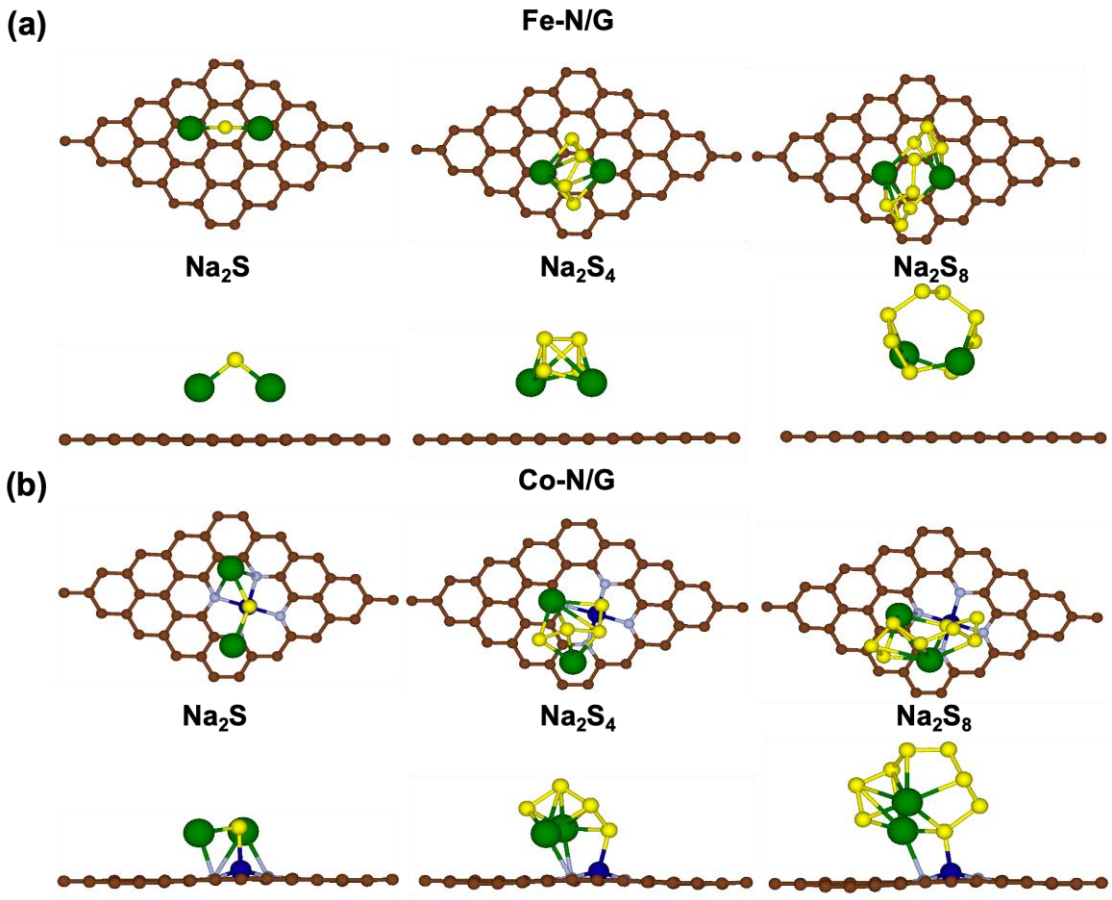

Figure S4. The top and side views of most stable geometric configurations of Na_2S_n (n = 1, 4 and 8) adsorbed (a) Fe and (b) Co@NG substrates.

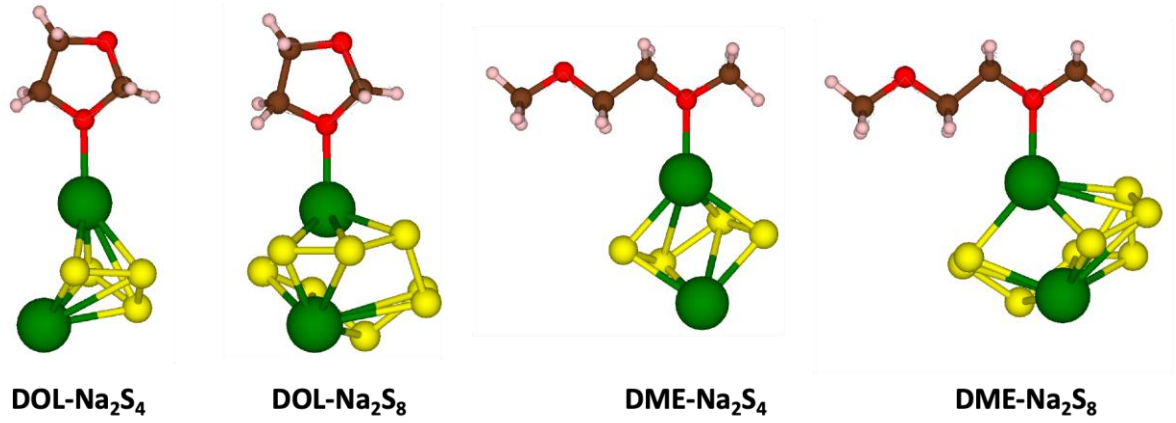

Figure S5. The optimized geometric configurations of Na_2S_n (n = 4 and 8) adsorbed DOL / DME electrolyte solvents

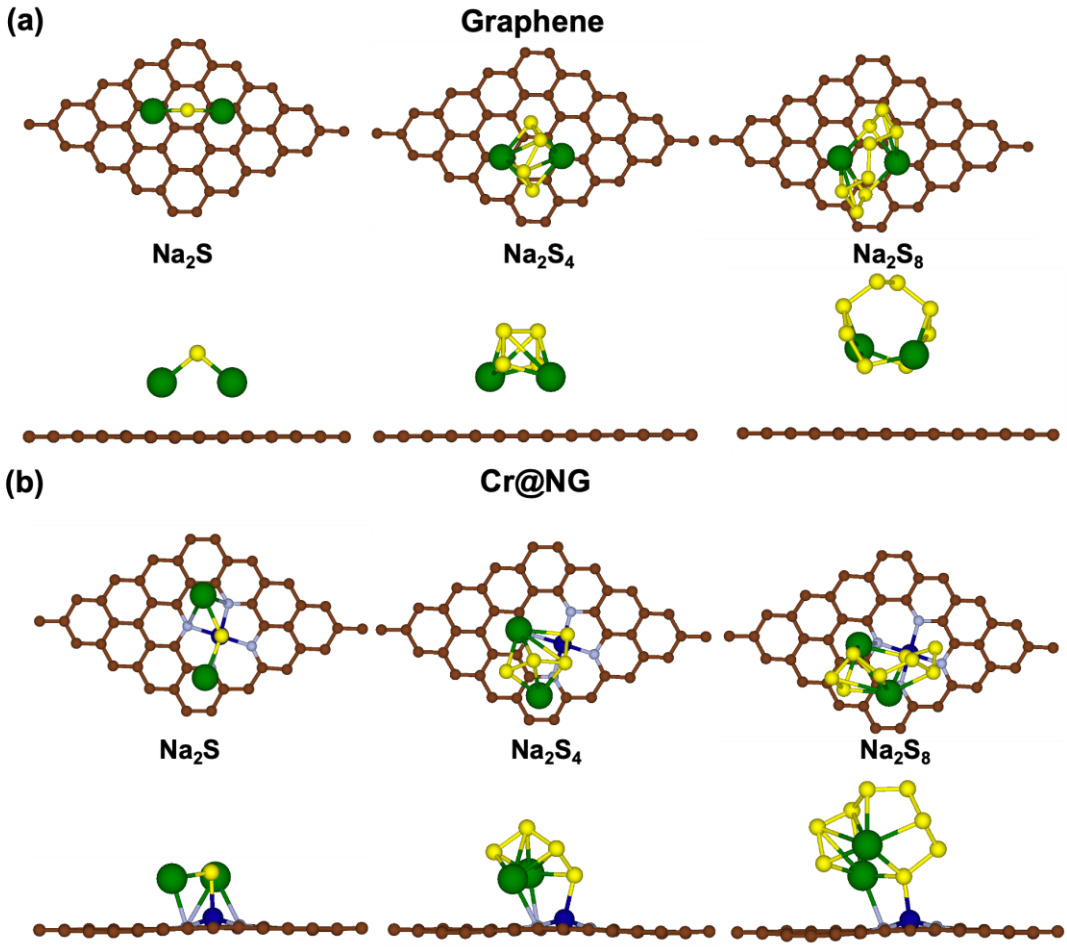

Figure S6. The top and side views of most optimized non-vdW adsorption configurations of Na_2S_n (n = 1, 4 and 8) adsorption on (a) graphene and (b) Cr@NG structures

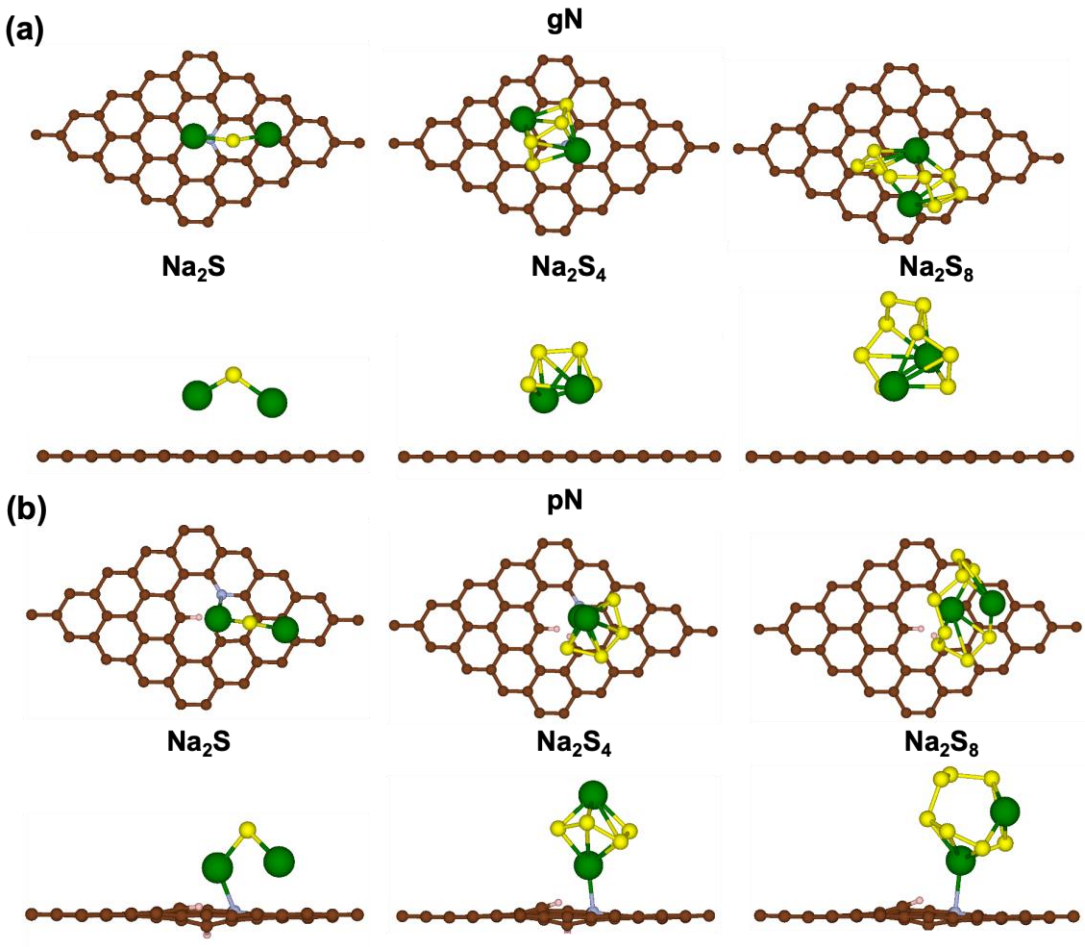

Figure S7. The top and side views of most stable non-vdW adsorption configurations of Na_2S_n where (n= 1, 4 and 8) adsorption on (a) gN and (b) pN.

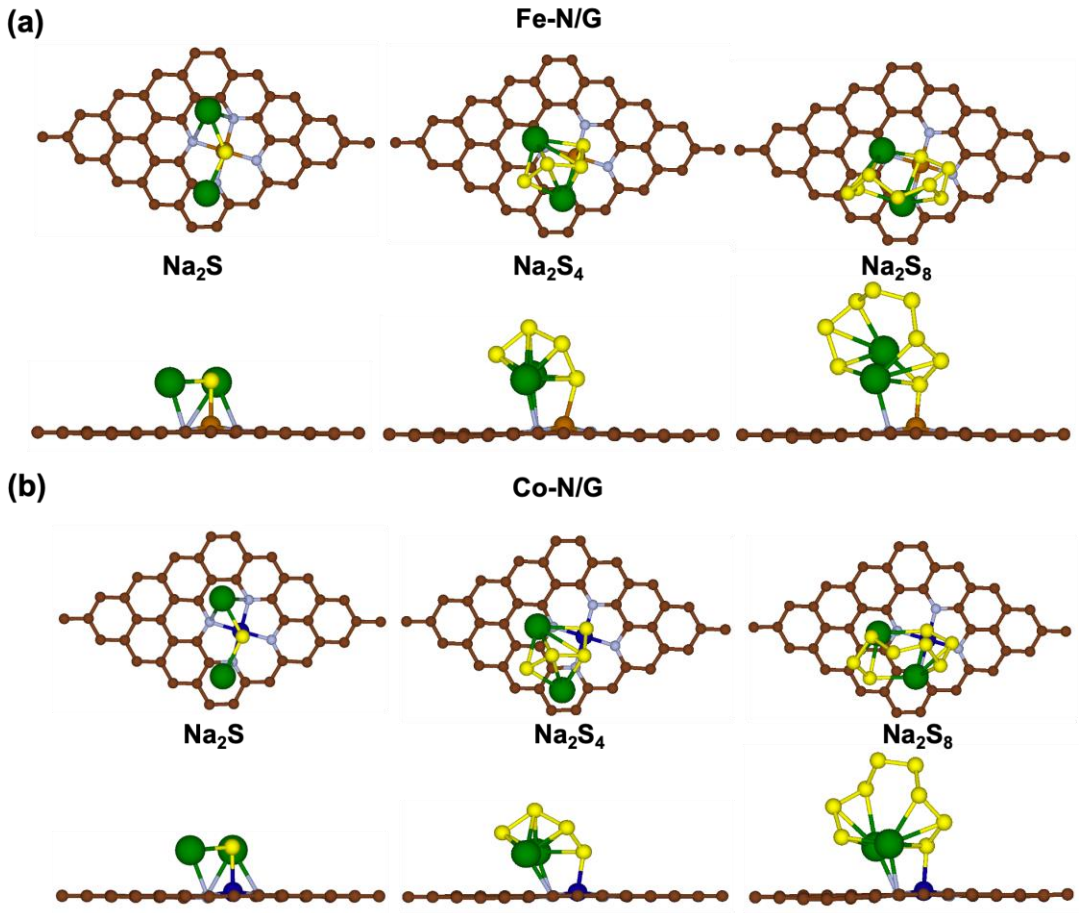

Figure S8. The top and side views of most optimized non-vdW adsorption configurations of Na_2S_n (n= 1, 4 and 8) adsorption on (a) Fe and (b) Co@NG structures

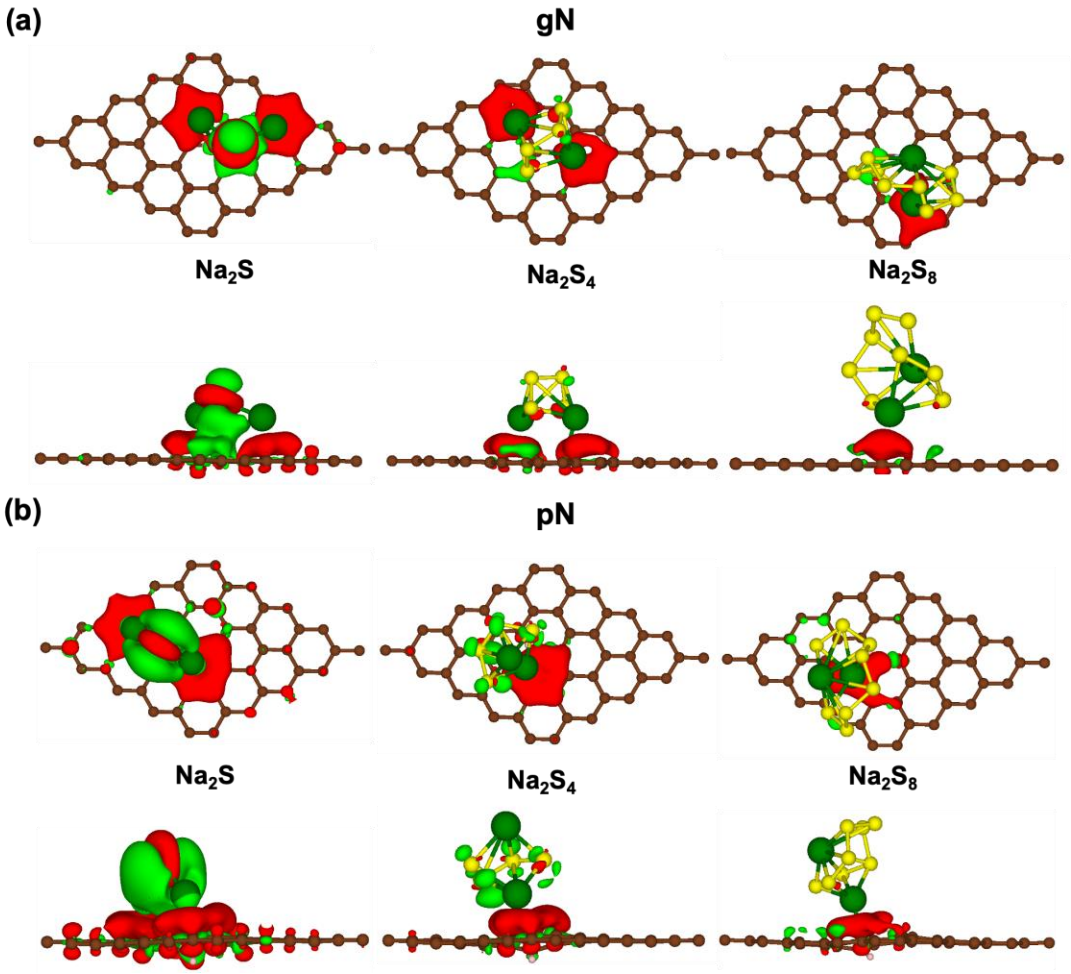

Figure S9. Charge density difference of Na_2S, Na_2S_4 and Na_2S_8 adsorbed (a) gN and (b) pN substrates. The iso-surface level is set at 0.001 e $Å^{-3}$. The green and red indicate charge depletion and accumulation respectively.

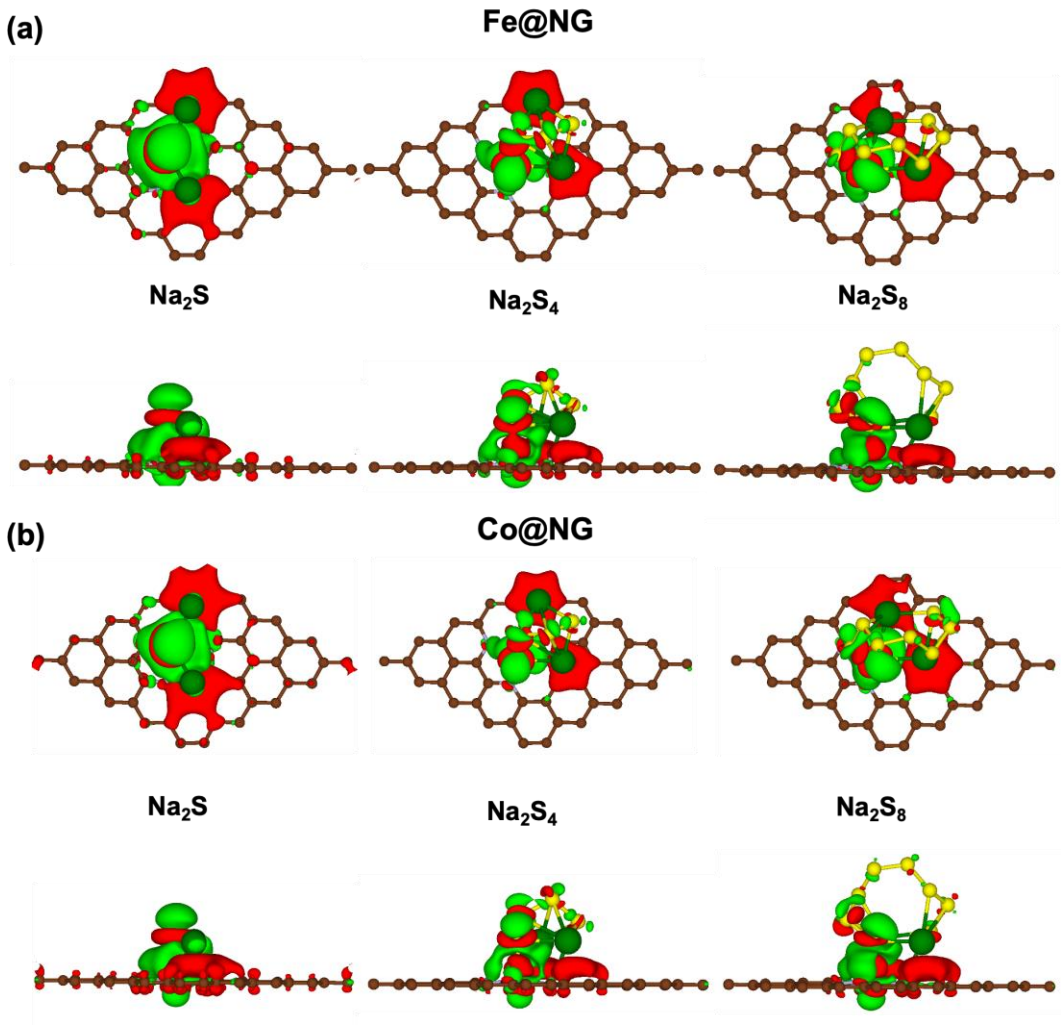

Figure S10. Charge density difference of Na_2S, Na_2S_4 and Na_2S_8 adsorbed (a) Fe and (b) Co@NG substrates. The iso-surface level is set at 0.001 e $Å^{-3}$. The green and red indicate charge depletion and accumulation respectively.

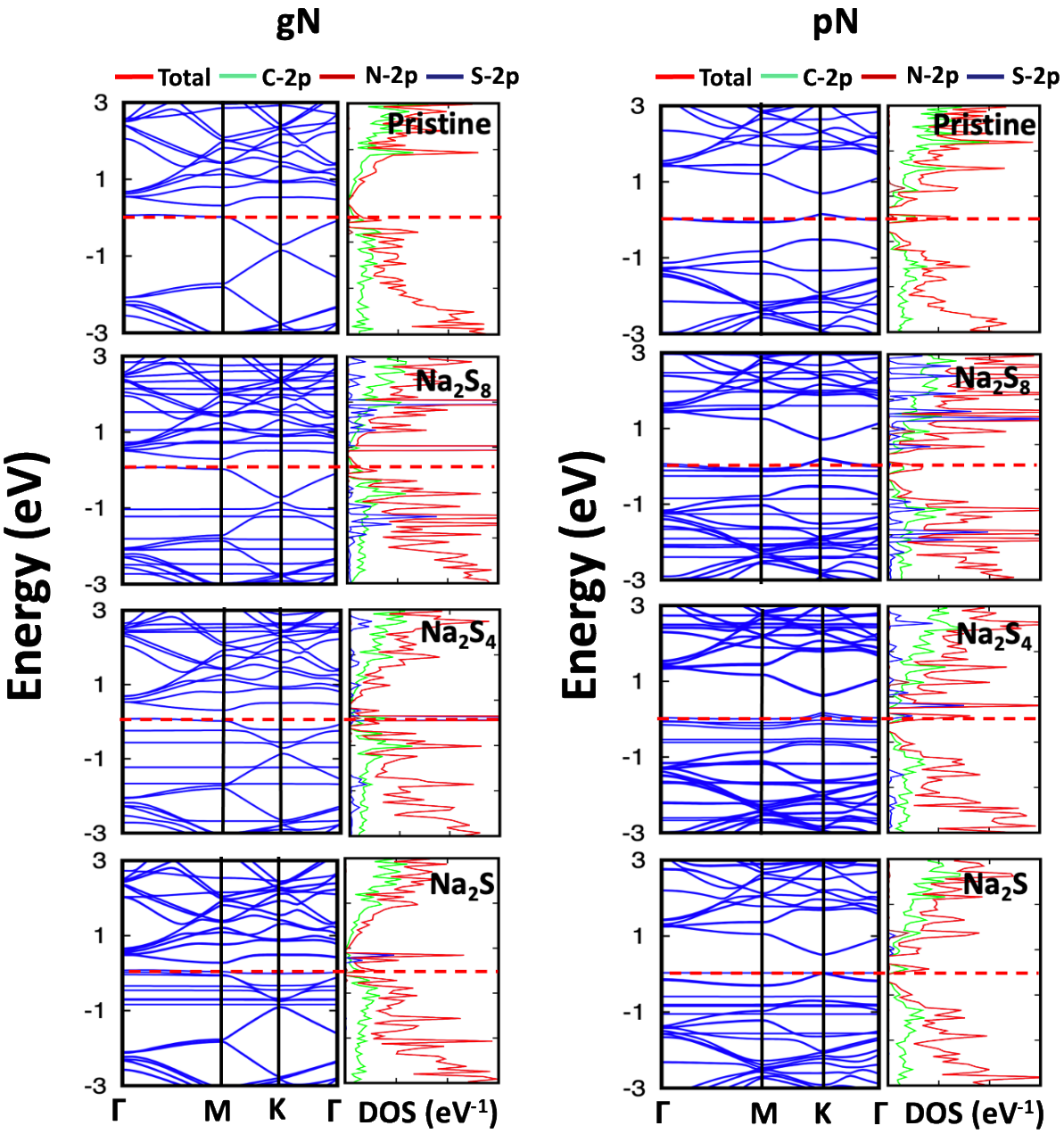

Figure S11. The computed band structure and projected density of states (PDOS) of pristine and various Na_2S_n species (n= 1, 4 and 8) adsorbed gN and pN substrates

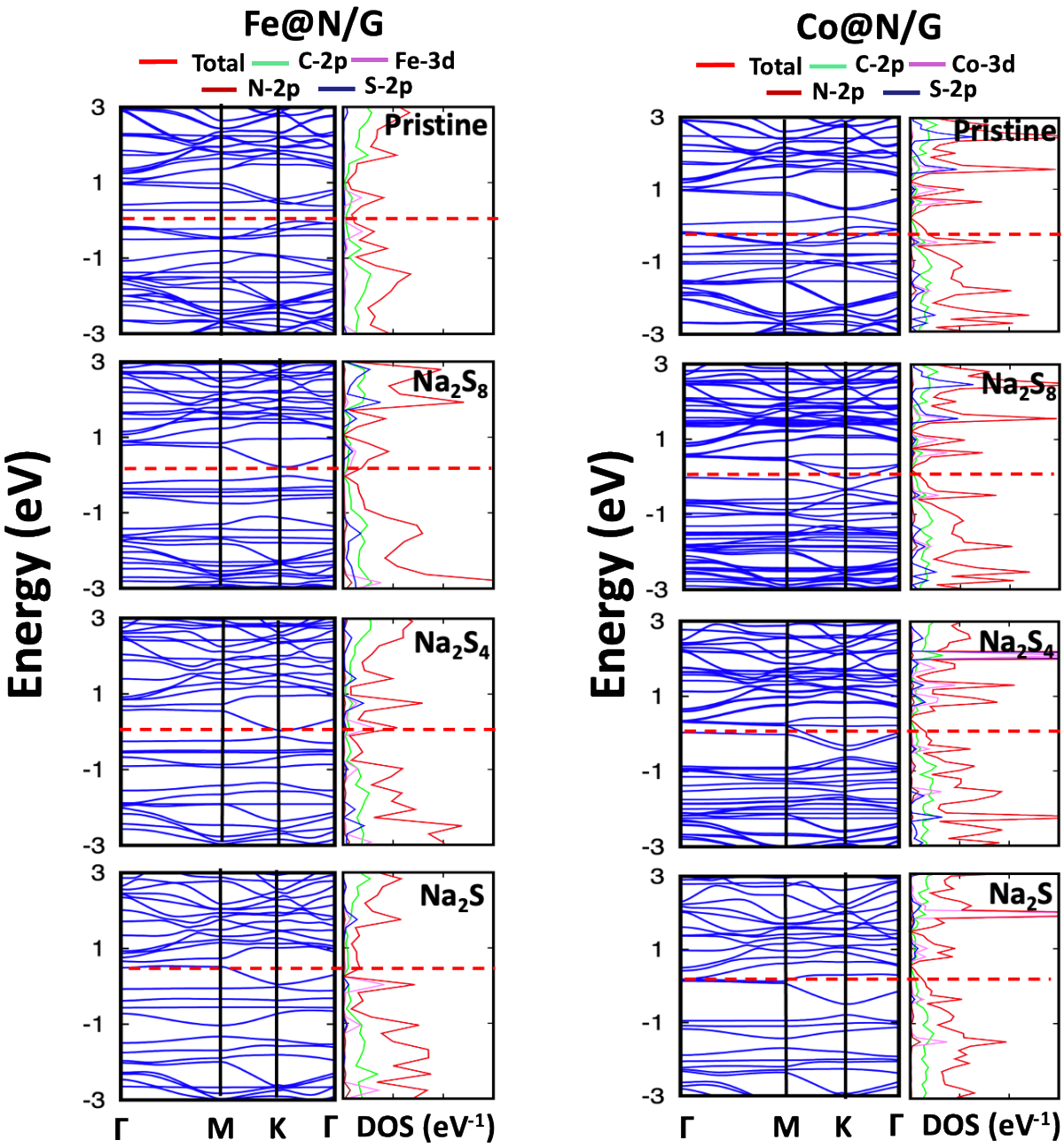

Figure S12. The computed band structure and projected density of states (PDOS) of pristine and various Na_2S_n species (n= 1, 4 and 8) adsorbed TM@NG (TM = Fe and Co) substrates

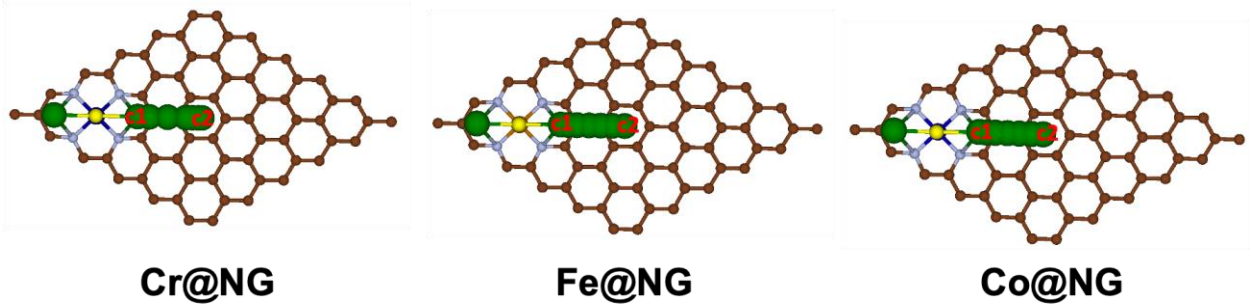

Figure S13. The path of Na_2S decomposition on TM@NG (where TM = Cr, Fe and Co) substrates. c1 and c2 represents favorable adsorption site 1 and 2.