

Mechanistic insights into the role of alkali metal activation in CO₂ adsorption by nitrogen-doped coal-based carbon materials

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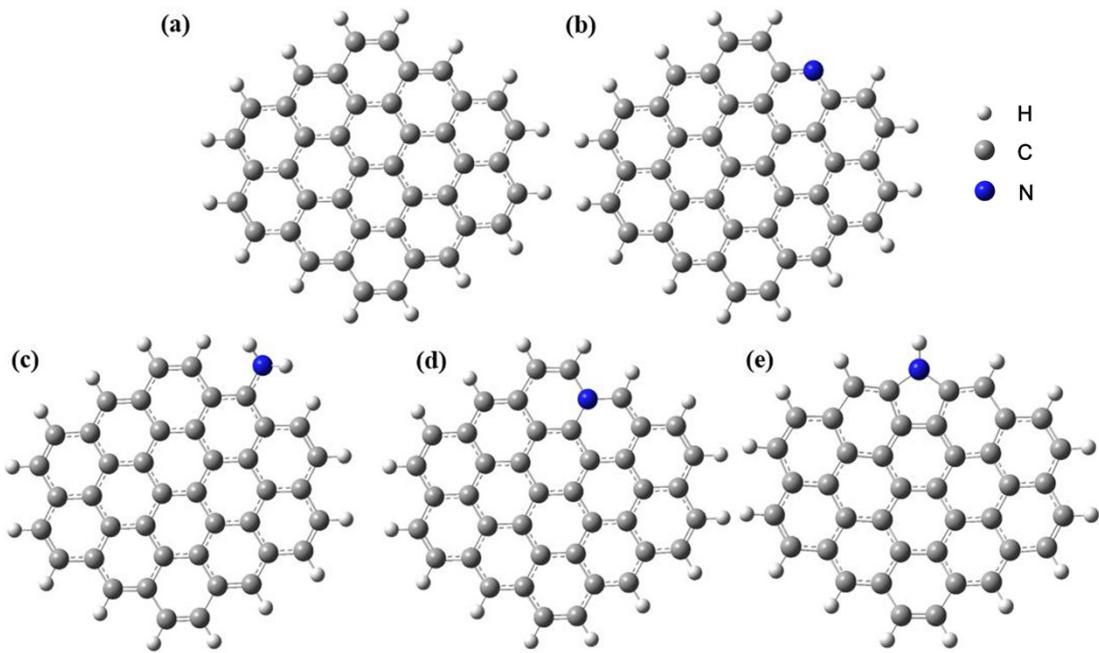


Figure S1 Nitrogen-doped carbon model (a) undoped carbon model; (b) Pyridine nitrogen-doped carbon model; (c) Amine-doped carbon model; (d) Graphite nitrogen-doped carbon model; (e) Pyrrole nitrogen-doped carbon model.

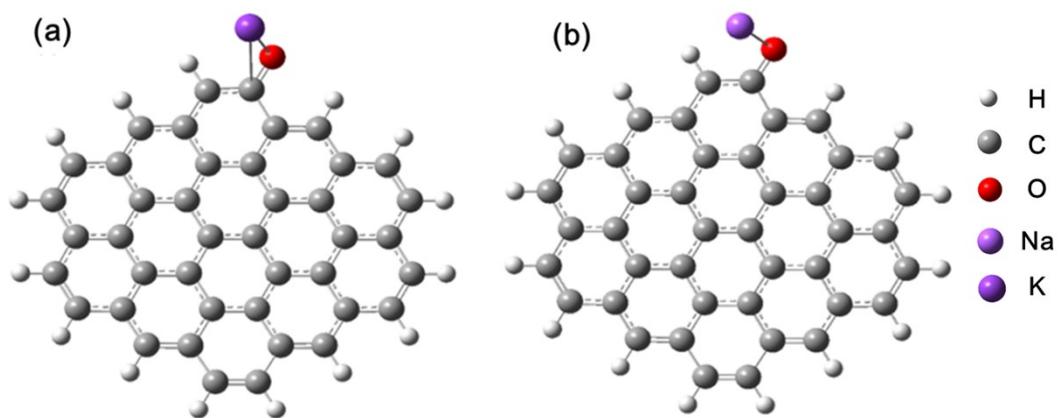


Figure S2 (a) K-doped activated carbon model; (b) Na-doped carbon model.

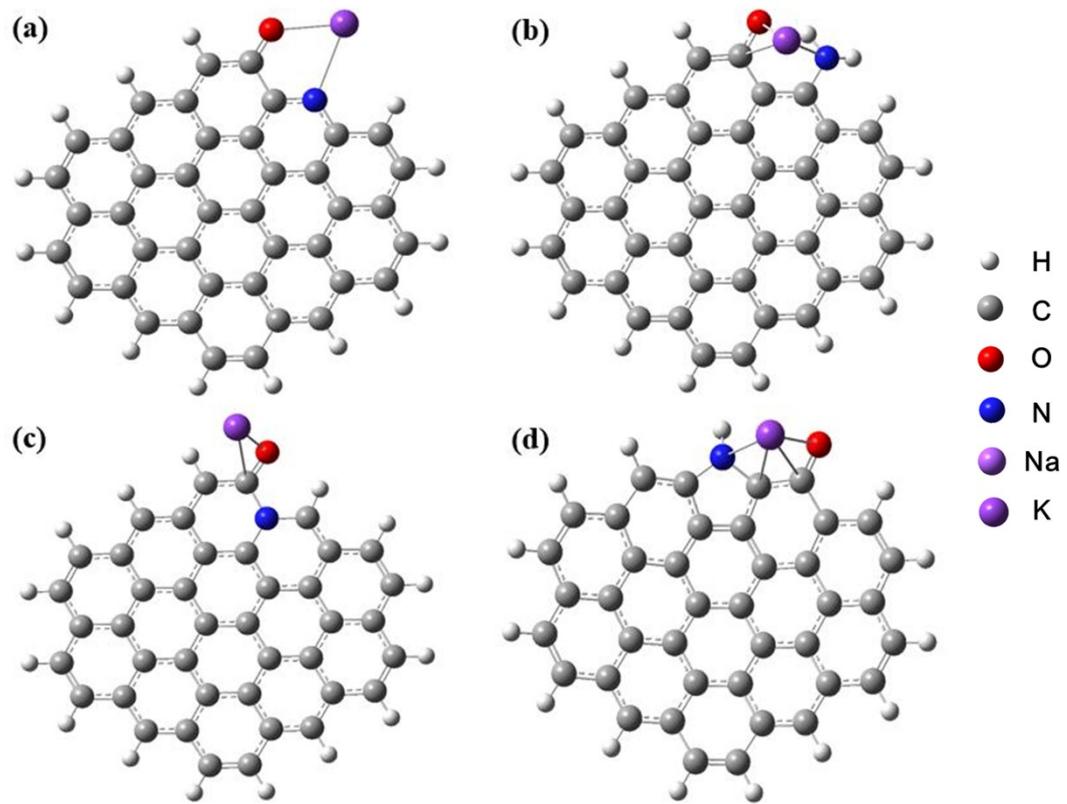


Figure S3 Various types of co-doped carbon models of N and alkali metals (K, Na). (a) Pyridine nitrogen; (b) Amino group; (c) Graphite nitrogen; (d) Pyrrole nitrogen.

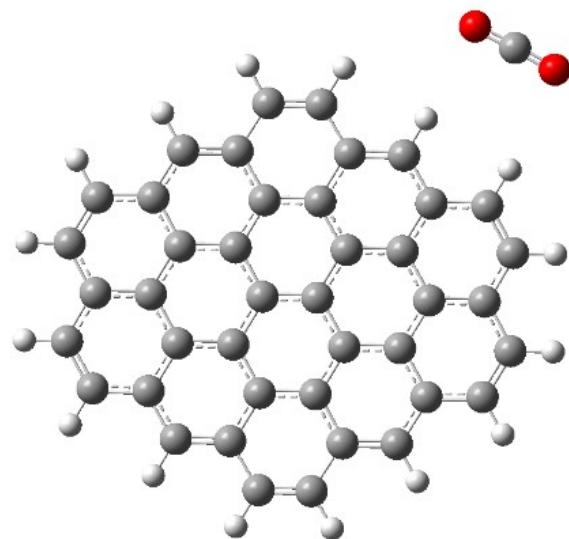


Figure S4 Adsorption configuration of CO₂ on the undoped carbon model.

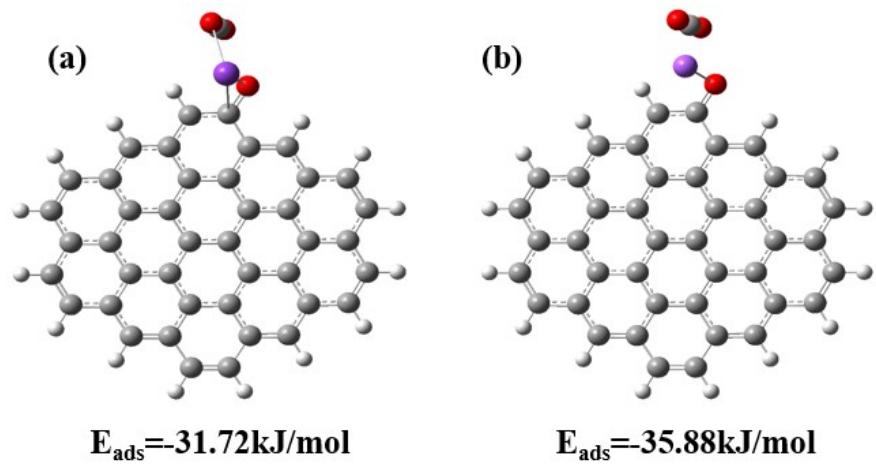


Figure S5 CO_2 adsorption configuration and adsorption energy on the surface of alkali metal-doped carbon (a)K doping (b)Na doping.

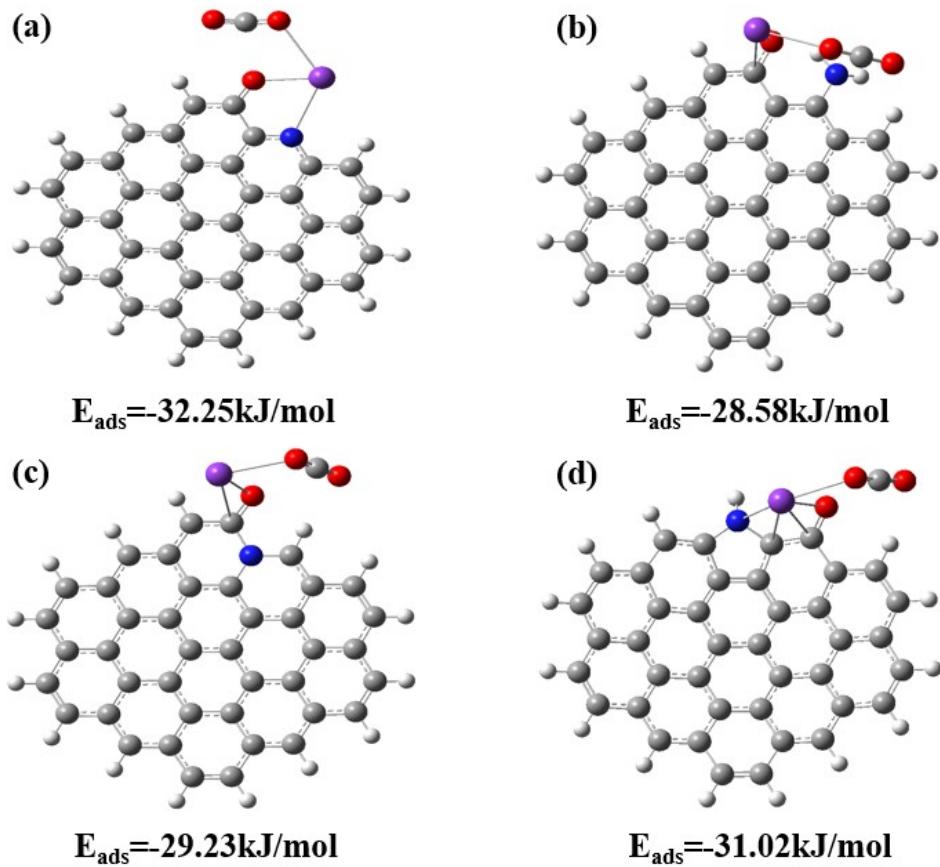


Figure S6 CO_2 adsorption configuration and adsorption energy of N and K co-doped carbon model (a) pyridine nitrogen; (b) Amino group; (c) Graphite nitrogen; (d) Pyrrole nitrogen.

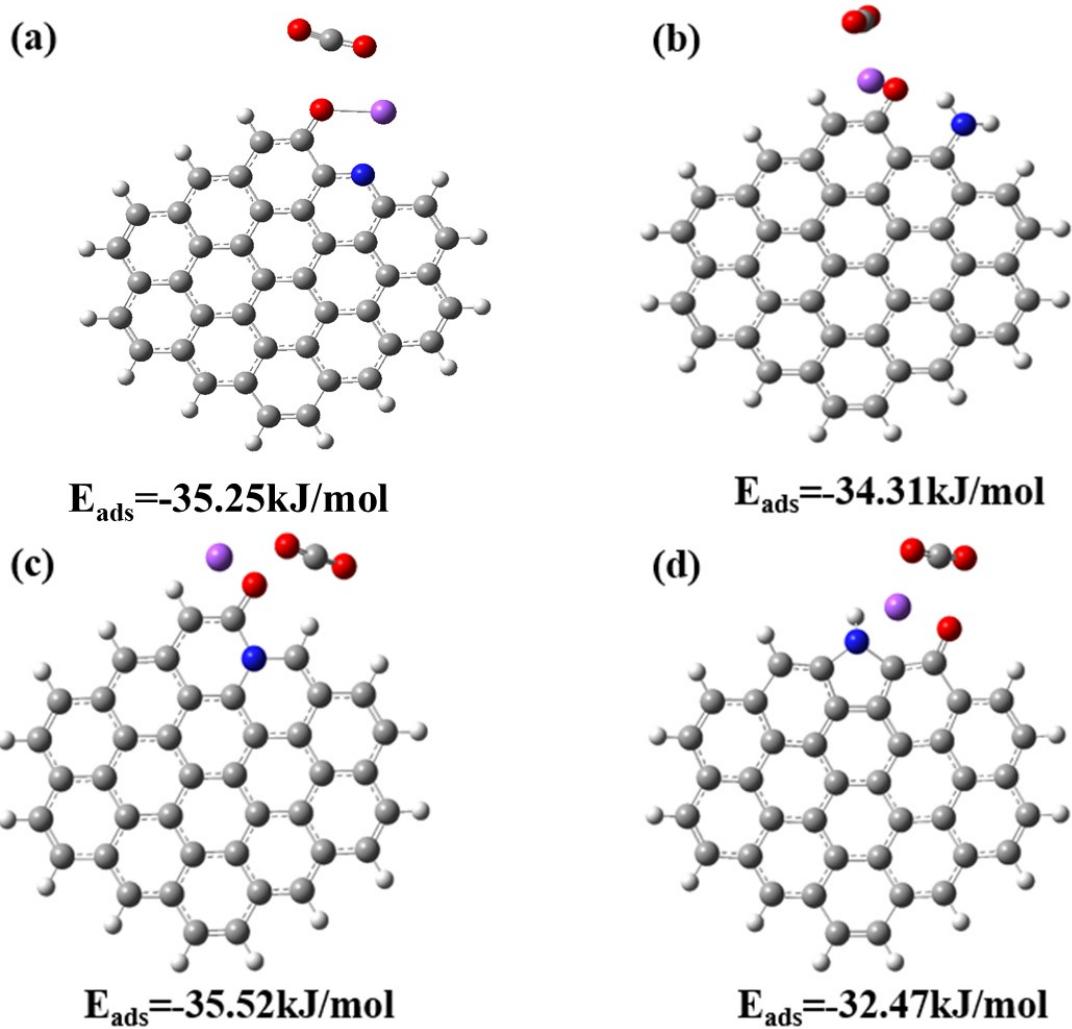


Figure S7 CO_2 adsorption configuration and adsorption energy of N and Na co-doped carbon model (a) pyridine nitrogen; (b) Amino group; (c) Graphite nitrogen; (d) Pyrrole nitrogen.

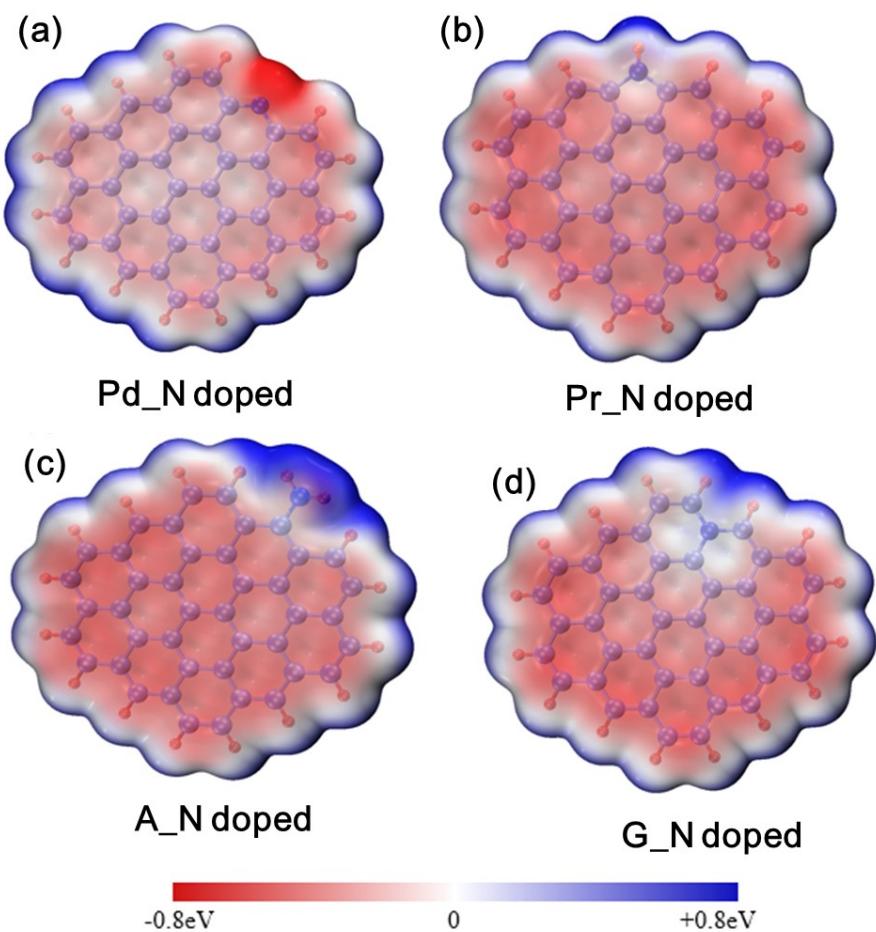


Figure S8 Electrostatic potential distribution diagram of the nitrogen-doped carbon model. (a) Pyridine nitrogen; (b) Pyrrole nitrogen; (c) amino group; (d) Graphite nitrogen.

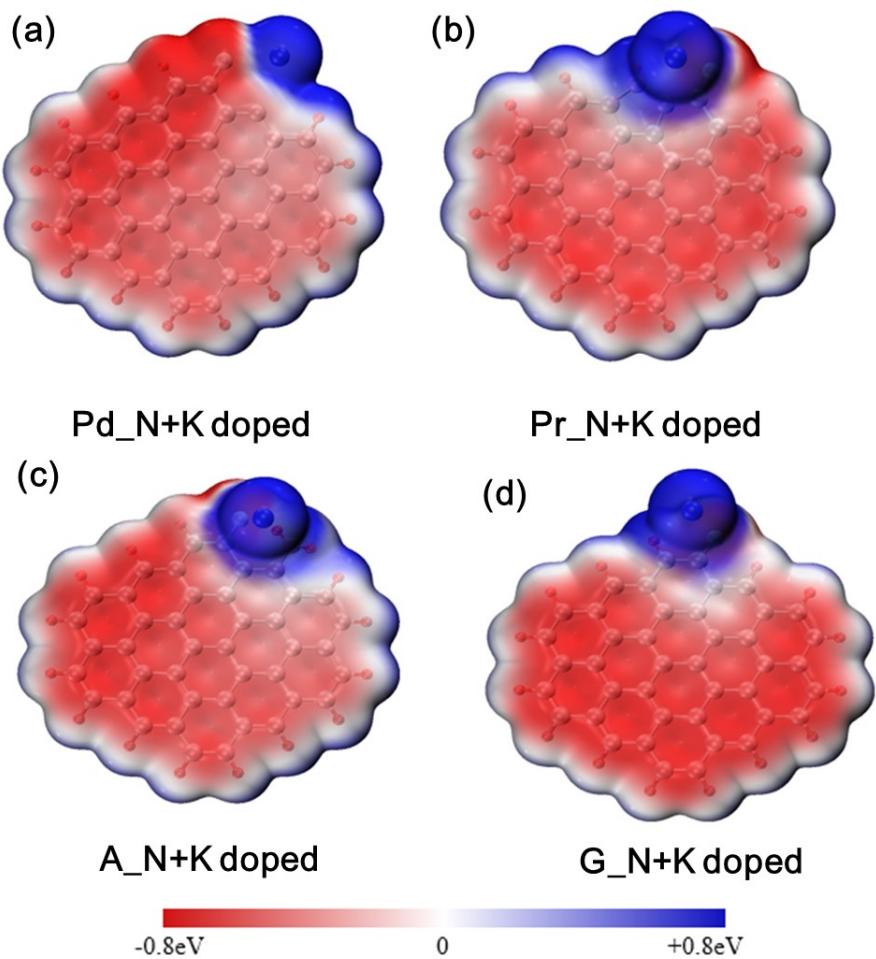


Figure S9 Electrostatic potential distribution of the nitrogen and potassium co-doped carbon model. (a) Pyridine nitrogen; (b) Pyrrole nitrogen; (c) amino group; (d) Graphite nitrogen.

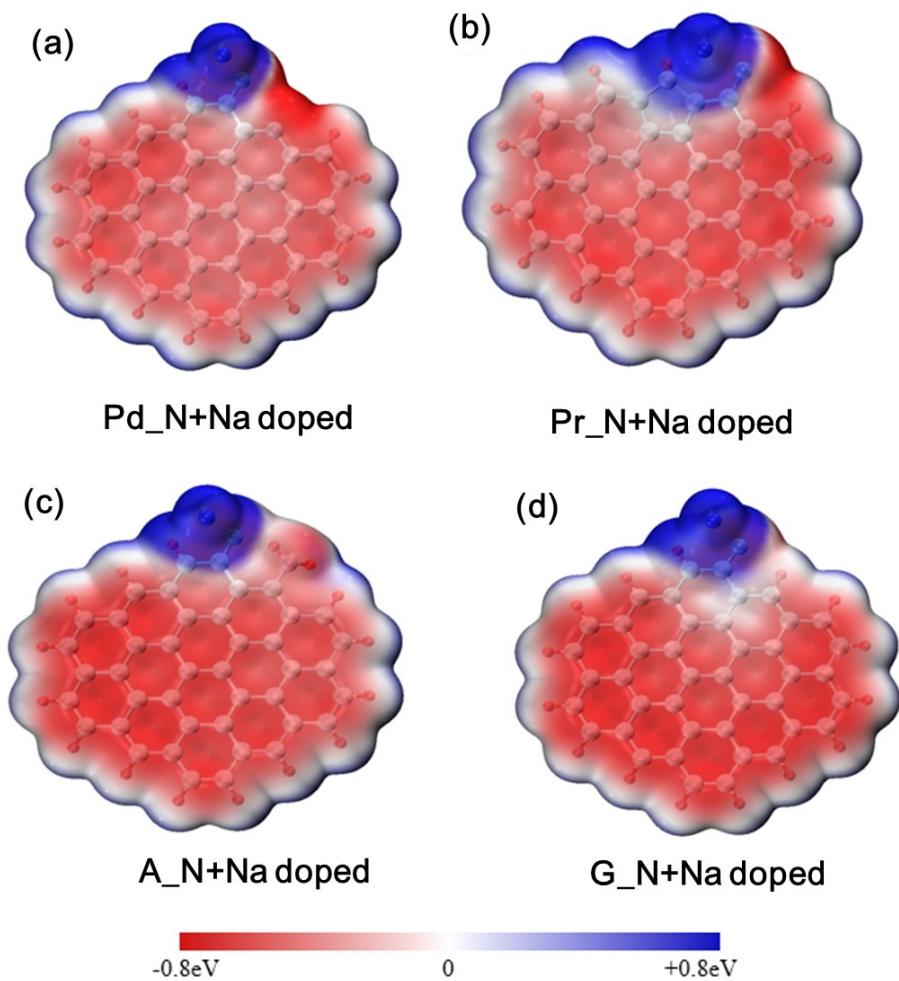


Figure S10 Electrostatic potential distribution of the carbon model co-doped with nitrogen and Na. (a) Pyridine nitrogen; (b) Pyrrole nitrogen; (c) amino group; (d) Graphite nitrogen.

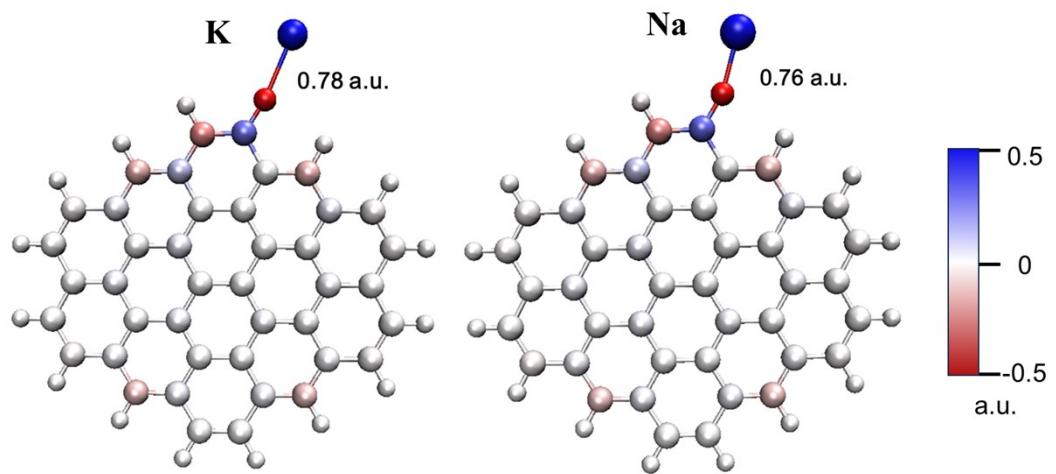


Figure S11 Mulliken population analysis of alkali metal (K, Na) doped carbon models.

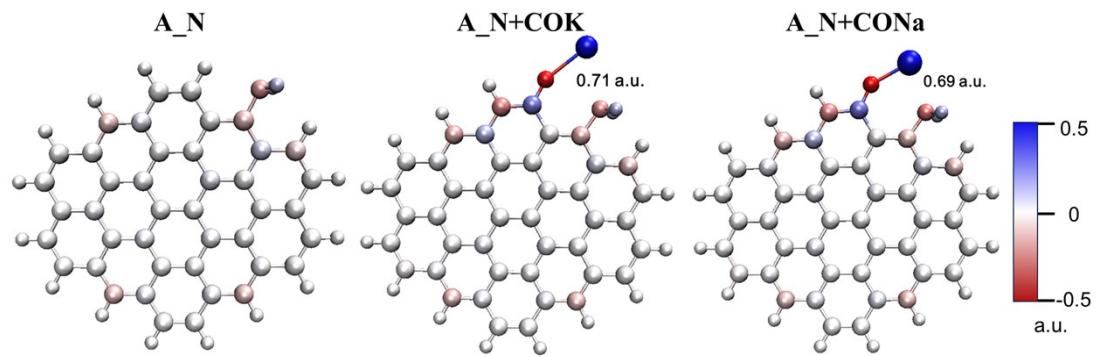


Figure S12 Mulliken population analysis of carbon models doped with amino, co-doped with amino and potassium, and co-doped with amino and sodium.

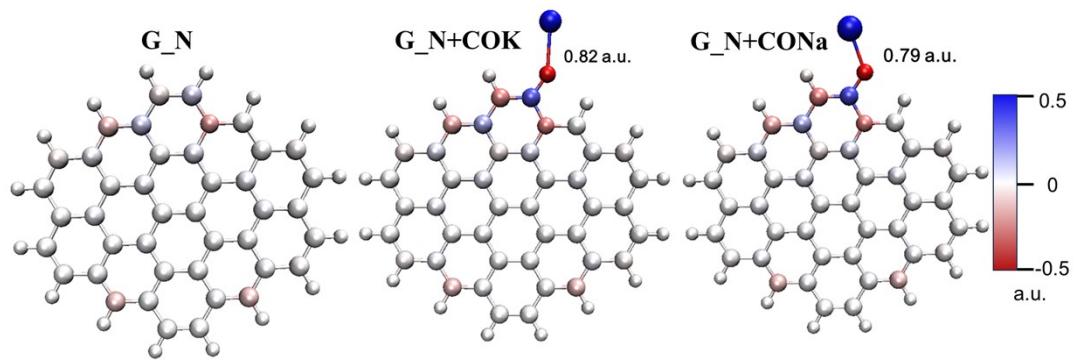


Figure S13 Mulliken population analysis of carbon models doped with graphite nitrogen, co-doped with graphite nitrogen and potassium, and co-doped with graphite nitrogen and sodium.

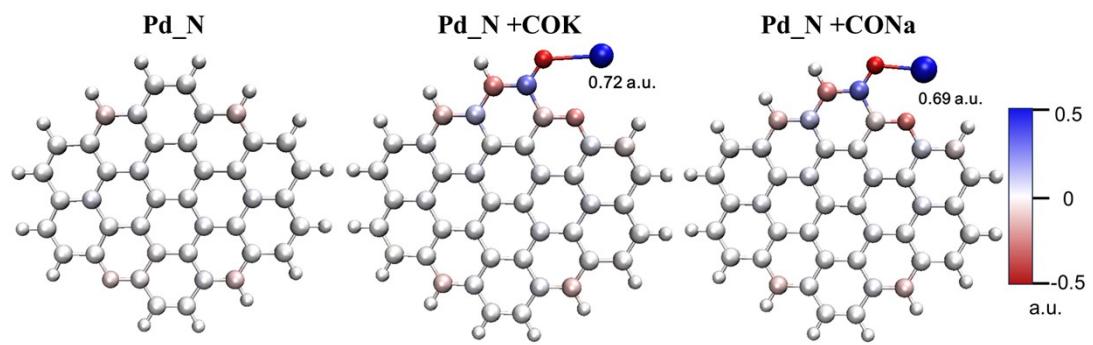


Figure S14 Mulliken population analysis of carbon models doped with pyridine nitrogen, co-doped with pyridine nitrogen and potassium, and co-doped with pyridine nitrogen and sodium.

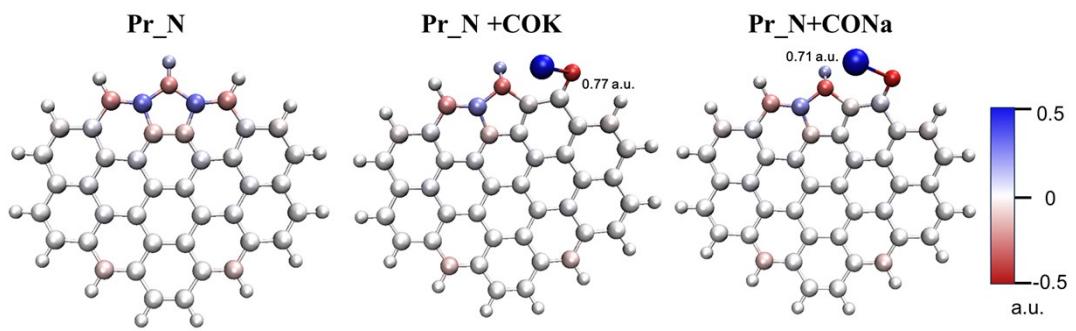


Figure S15 Mulliken population analysis of carbon models doped with pyrrole nitrogen, co-doped with pyrrole nitrogen and potassium, and co-doped with pyrrole nitrogen and sodium.

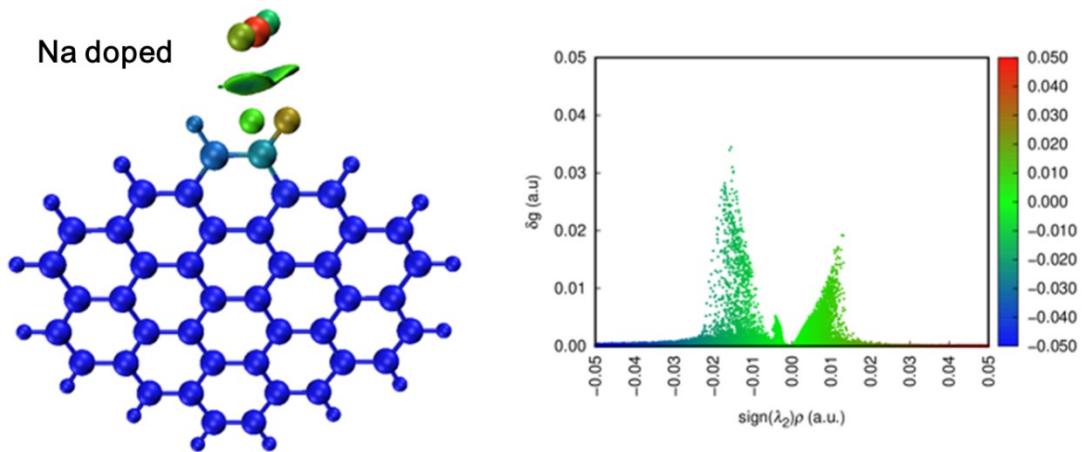


Figure S16 IGMH analysis diagram of CO₂ adsorption on the surface of the Na-doped carbon model.

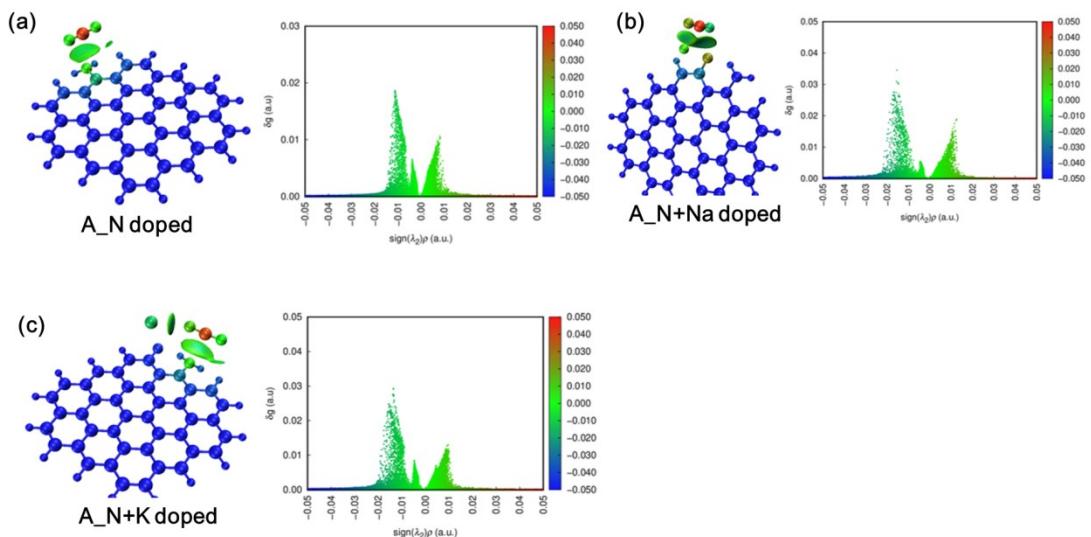


Figure S17 IGMH analysis diagram of CO₂ adsorption on the surface of the carbon model co-doped with amino and alkali metals. (a) Amino doping; (b) Co-doping of amino and Na; (c) The amino group and K are co-doped.

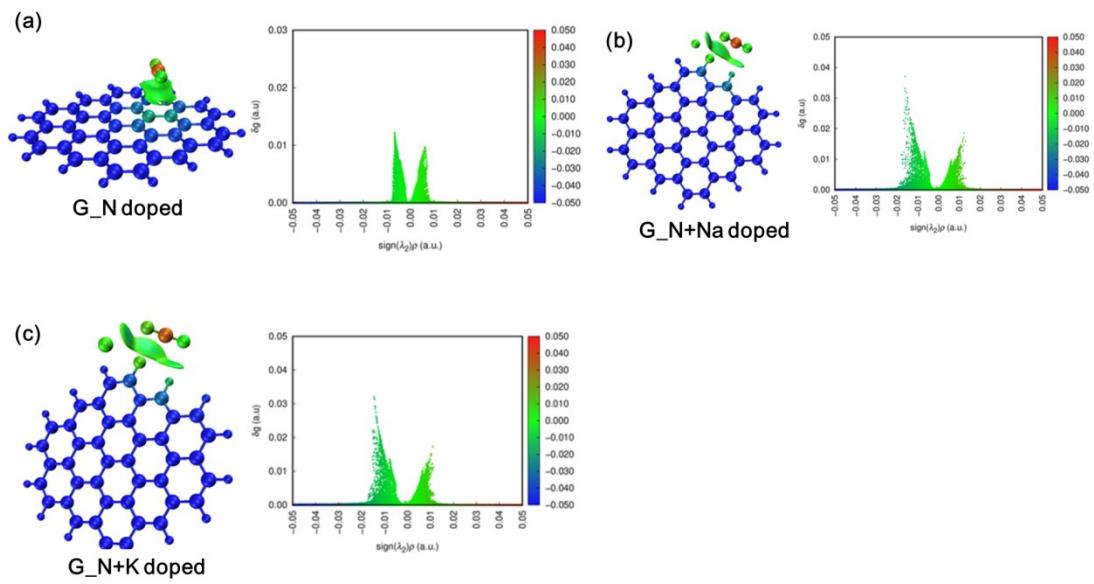


Figure S18 IGMH analysis diagram of CO₂ adsorption on the surface of the graphite nitrogen and alkali metal co-doped carbon model. (a) Graphite nitrogen doping; (b) Graphite nitrogen and Na co-doped; (c) Graphite nitrogen and K co-doped.

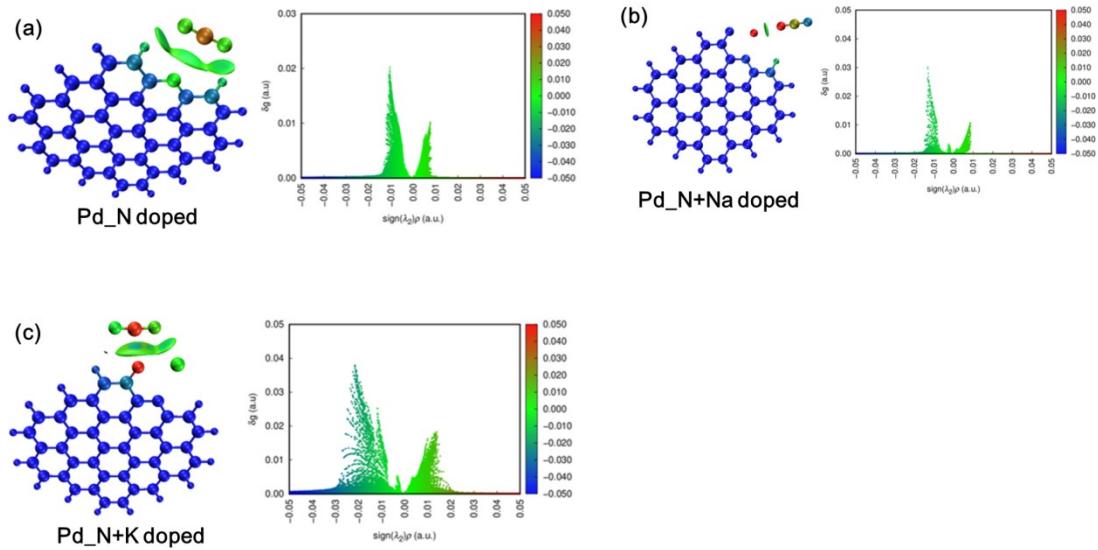


Figure S19 IGMH analysis diagram of CO₂ adsorption on the surface of the carbon model co-doped with pyridine nitrogen and alkali metals. (a) Pyridine nitrogen doping; (b) Co-doping of pyridine nitrogen and Na; (c) Pyridine nitrogen and K are co-doped.

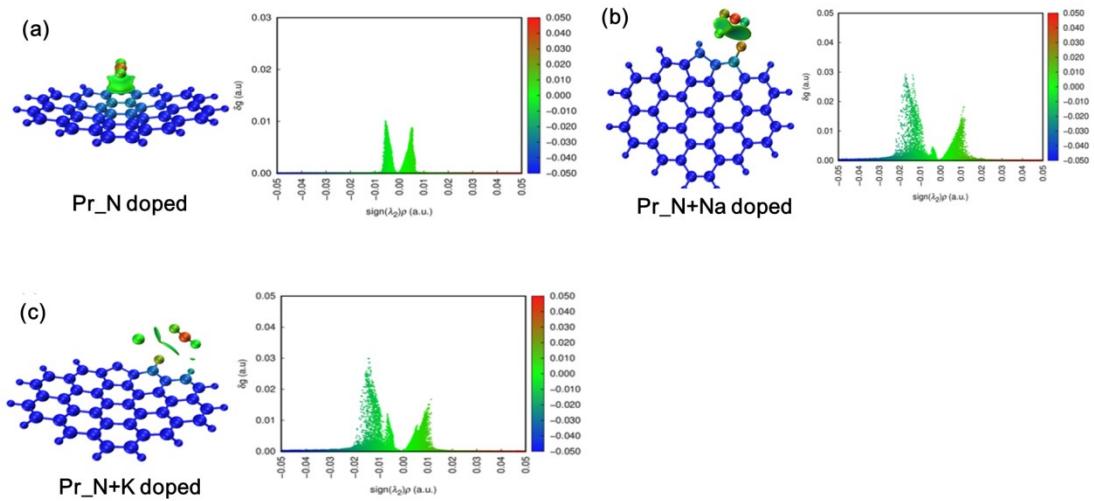


Figure S20 IGMH analysis diagram of CO_2 adsorption on the surface of the carbon model co-doped with pyrrole nitrogen and alkali metals. (a) pyrrole nitrogen doping; (b) Co-doping of pyrrole nitrogen and Na; (c) Pyrrole nitrogen and K are co-doped.