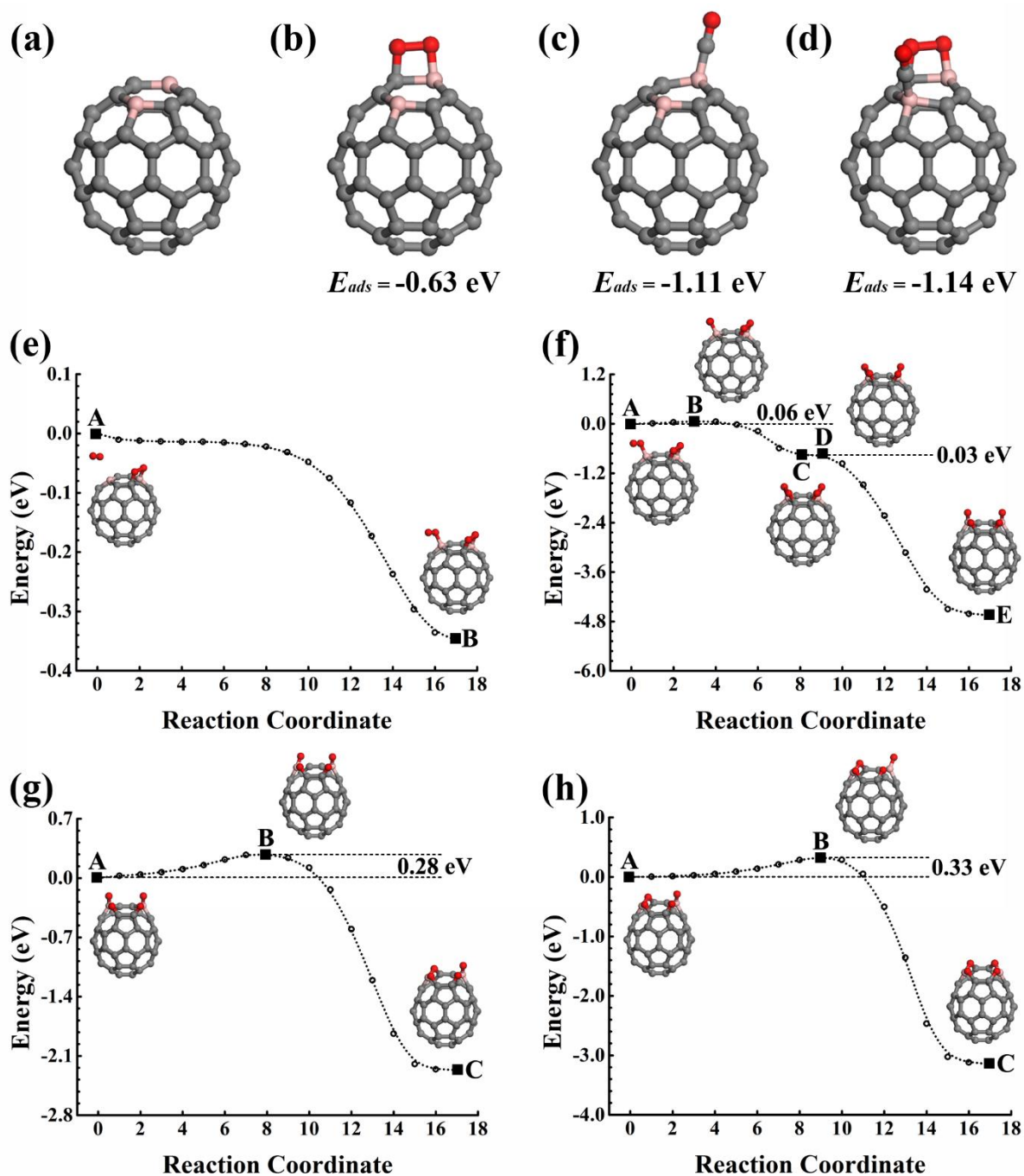
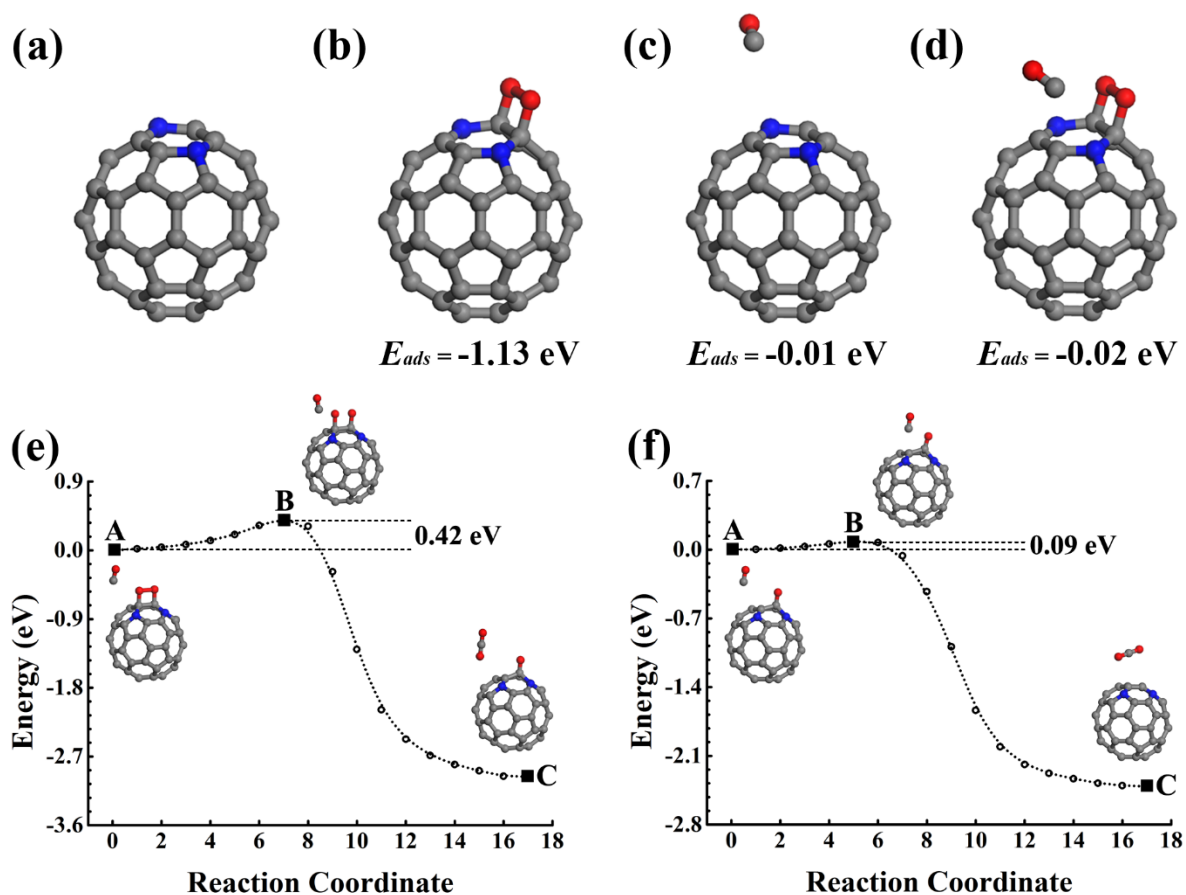


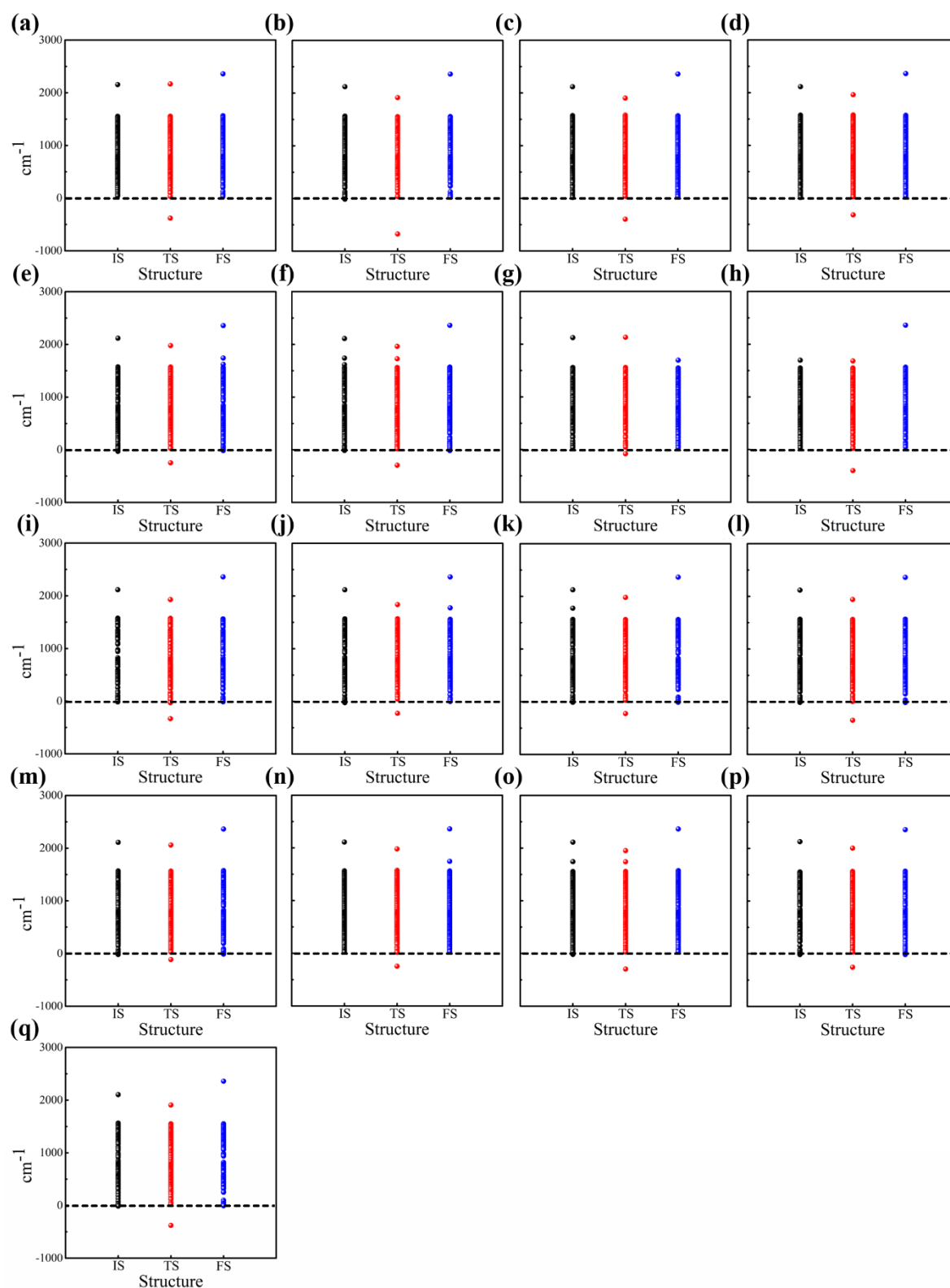
## Supplemental Materials



**Figure S1** (a)-(d) are structures of two B atoms doped fullerenes and the corresponding gas molecule adsorption configurations on  $C_{58}B_2$ . The adsorption energies are given too. (e)-(h) show the reaction paths of  $C_{58}B_2$  oxidation. The C, B, and O accounted by the grey, pink, and red balls.



**Figure S2** (a)-(d) are structures of two N atoms doped fullerenes and the corresponding gas molecule adsorption configurations on  $C_{58}N_2$ . The adsorption energies are given too. (e) and (f) are the reaction paths of CO oxidizations catalyzed by  $C_{58}N_2$ . The C, N, and O accounted by the grey, blue, and red balls.



**Figure S3** The frequencies of initial state (IS), rate-determining transition state (TS), and final state (FS) structures studied in the manuscript. Black, red, blue dots stand for IS, TS, and FS, respectively. (a), (b) correspond to Fig. 1g and 1h; (c)-(h) correspond to Fig.2g-2l; (i)-(k) correspond to Fig.3d-3f; (l) and (m) correspond to Fig. 4f and 4g; and (n)-(q) correspond to Fig. 5f-5i, respectively.