CO_2 Adsorption Thermodynamics over N-substituted/grafted Graphanes: a DFT Study

Jing Xiao[a], Siddarth Sitamraju[b], Michael J. Janik[b,c]*

[a] Key Laboratory of Heat Transfer Enhancement and Energy Conservation of Education Ministry, and School of Chemistry and Chemical Engineering, South China University of Technology, Guangzhou 510640, China

[b] EMS Energy Institute, the Pennsylvania State University, University Park, PA 16802, U.S.

[c] Department of Chemical Engineering, the Pennsylvania State University, University Park, PA 16802, U.S.

Corresponding Author: *E-mail: cejingxiao@scut.edu.cn (J.X.)

Supporting Information

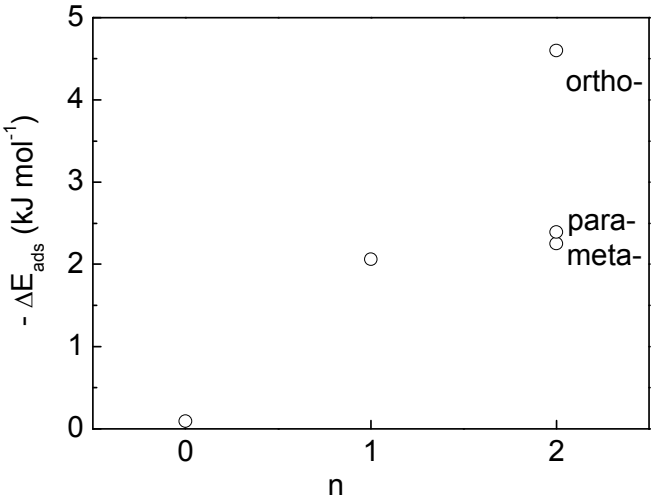

Figure S1. CO_2 adsorption energy versus degree of N-substitution in a 4×4 graphane unit cell.