Computational Materials Science 239 (2024) 112921

Contents lists available at ScienceDirect

Computational Materials Science

journal homepage: www.elsevier.com/locate/commatsci

Corrigendum

Corrigendum to "Functionalized carbophenes as high-capacity versatile gas adsorbents: An ab initio study" [Comput. Mater. Sci. 232 (2023) 112665]

Chad E. Junkermeier [a,b,*], Evan Larmand [c], Jean-Charles Morais [c], Jedediah Kobebel [b], Kat Lavarez [a], R. Martin Adra [a], Jirui Yang [a], Valeria Aparicio Diaz [a], Ricardo Paupitz [d], George Psofogiannakis [c]

[a] Department of Physics and Astronomy, University of Hawai'i at Mānoa, Honolulu HI 96822, USA
[b] Science, Technology, Engineering, and Mathematics Department, University of Hawai'i Maui College, Kahului HI 96732, USA
[c] Department of Chemical and Biological Engineering, University of Ottawa, Ottawa, Ontario, Canada
[d] Departamento de Física, IGCE, Universidade Estadual Paulista, UNESP, 13506-900, Rio Claro, SP, Brazil

The authors have identified errors in Figures 6 and 9 of that publication. The wrong CO_2 total energy was used when calculating adsorption energies in Equation 2 of that publication, resulting in the DFTB+-based CO_2 adsorption energies being too large by 0.1347 eV. The corrected graphs are given as Figures 1 and 2 of this corrigendum.

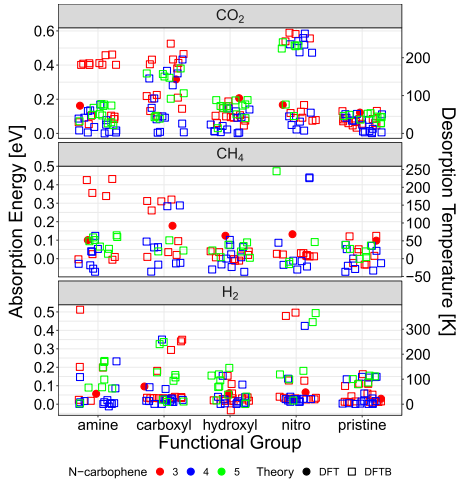

Figure 1. Corrected Figure 6.

.

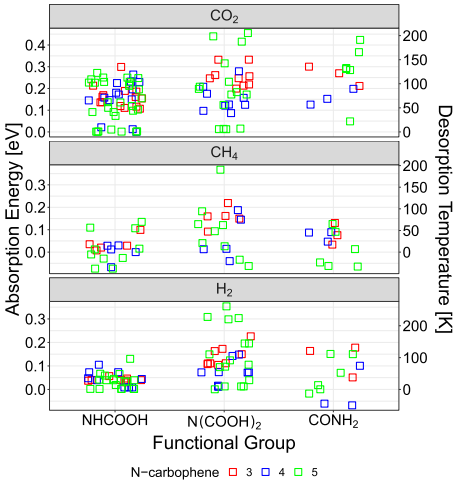

Figure 2. Corrected Figure 9.

The authors would like to apologise for any inconvenience caused.

DOI of original article: https://doi.org/10.1016/j.commatsci.2023.112665.
* Corresponding author at: Department of Physics and Astronomy, University of Hawai'i at Mānoa, Honolulu HI 96822, USA.
E-mail address: junkerme@hawaii.edu (C.E. Junkermeier).

https://doi.org/10.1016/j.commatsci.2024.112921

Available online 25 March 2024