

Computational Investigation of Stability and Reactivity of Edge Effect in Biochar Using DFT

T.K. Gunawardhana¹², B.S.W. Karunarathna^{12*}, A.S. Dahanayake², L. Karunanayake¹², and T. Etampawala^{12*}

¹Center for Nanocomposite Research, Faculty of Applied Sciences, University of Sri Jayewardenepura, Nugegoda 10250, Sri Lanka, ²Department of Polymer Science, Faculty of Applied Sciences, University of Sri Jayewardenepura, Nugegoda 10250, Sri Lanka

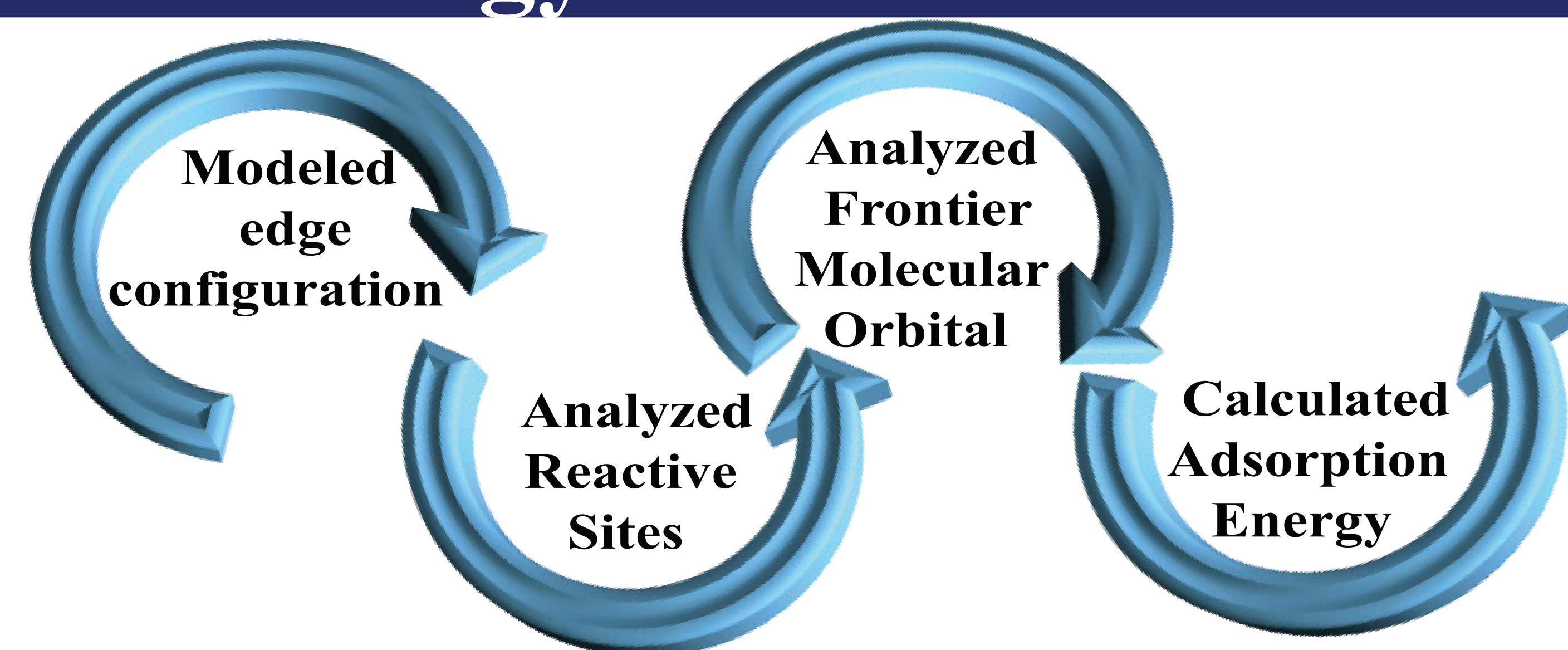
*Corresponding Author: tetampa@sjp.ac.lk

*Co-corresponding Author: baggya.karunarathna@gmail.com

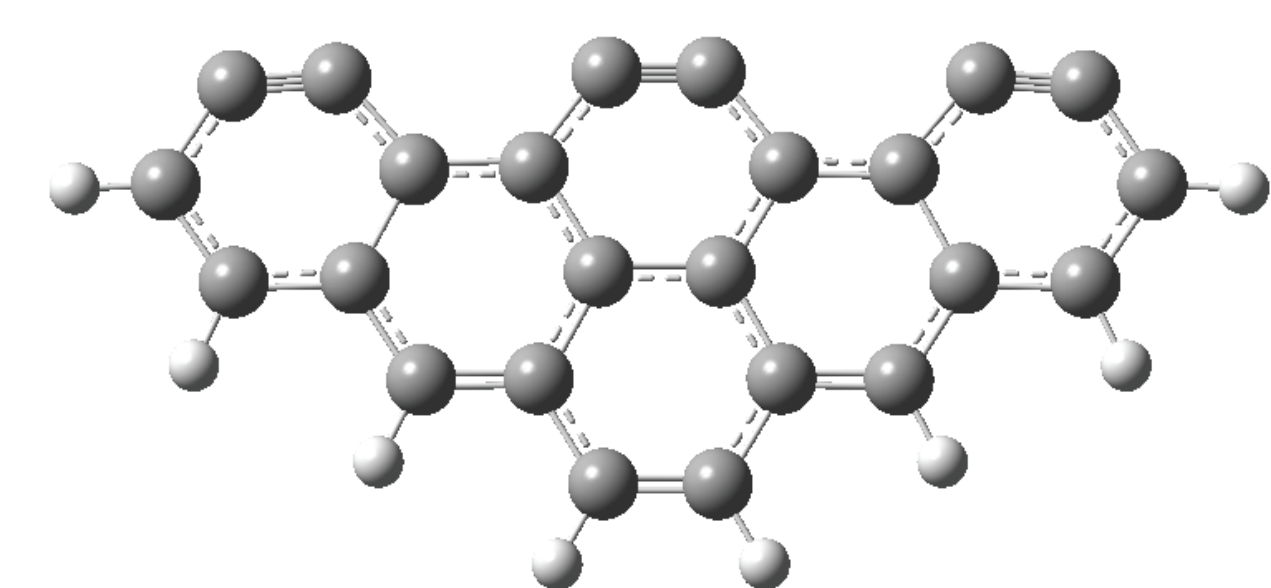
Introduction

Biochar (BC) is a carbon-rich solid produced through the thermal decomposition of biomass under limited or oxygen-free conditions. BC has several applications in soil amendment, water retention, energy storage. BC edges mainly exist as armchair, and zigzag configurations, which strongly influence the surface reactivity.

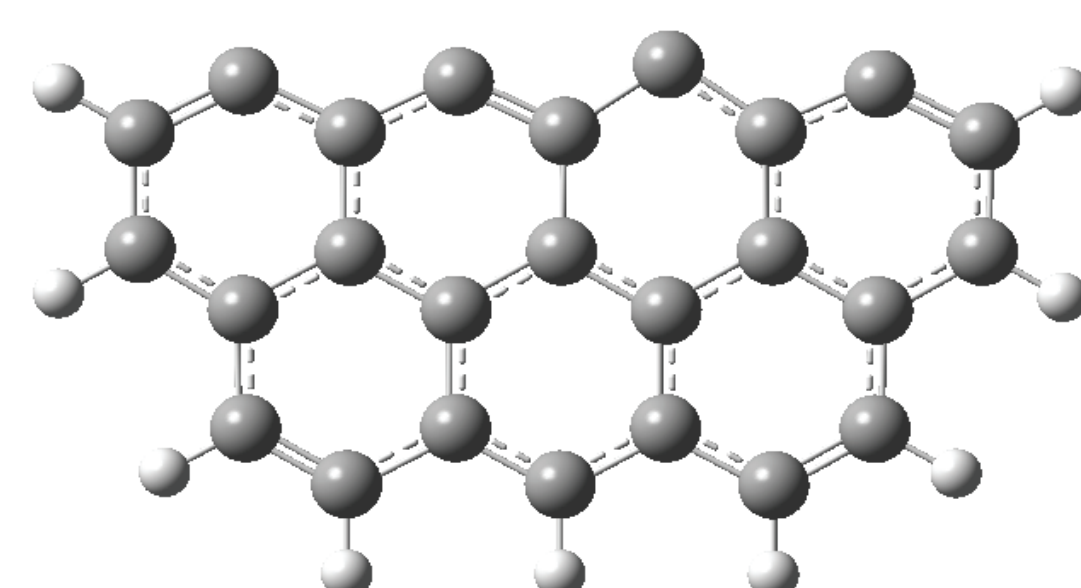
Methodology



Results and Discussion

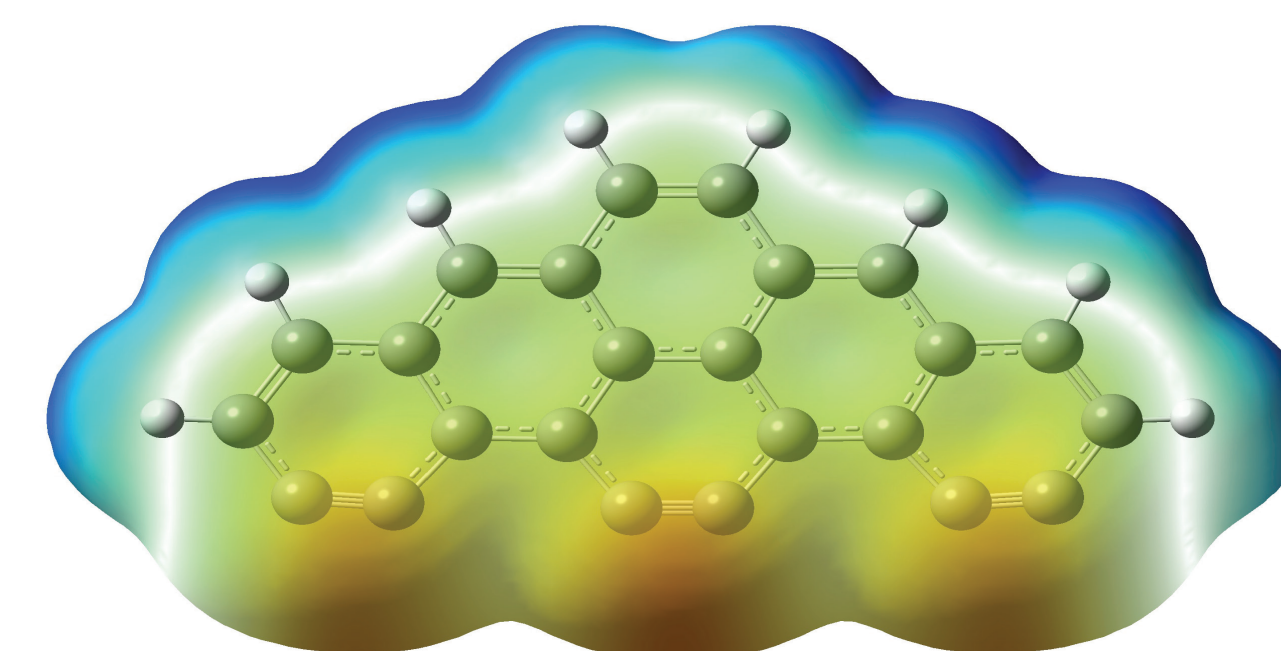


armchair configuration

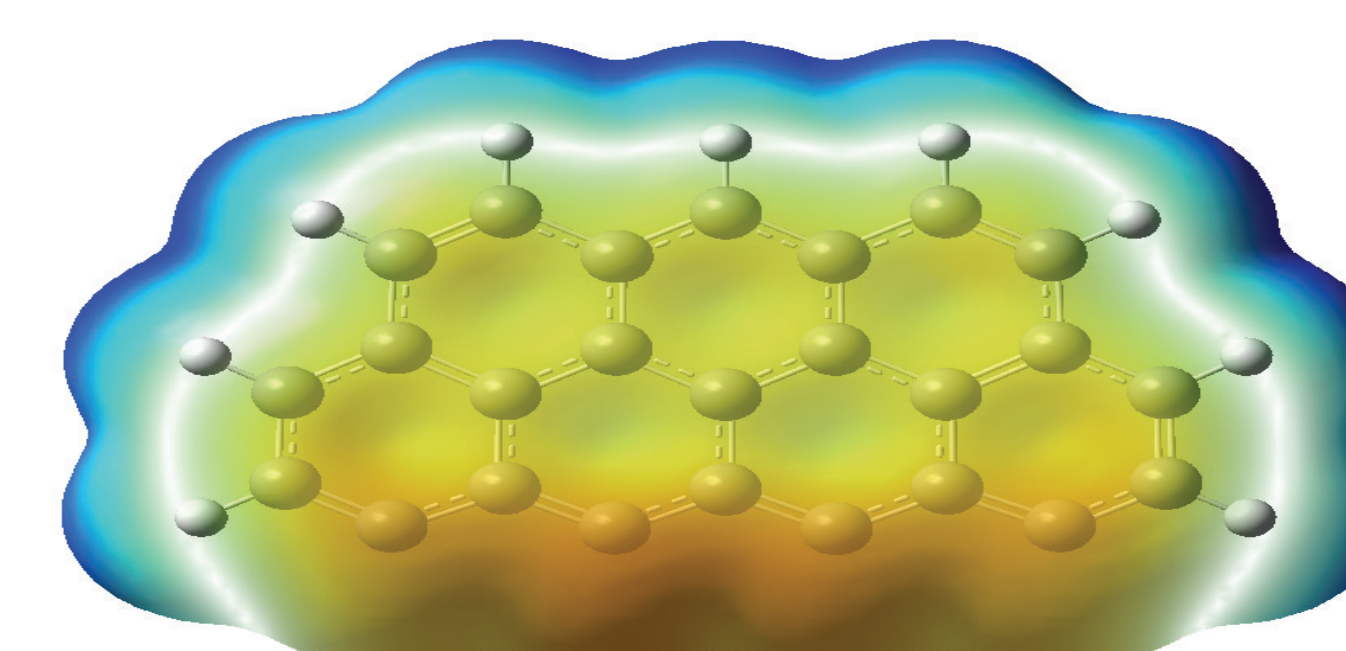


zig-zag configuration

Electrostatic Potential (ESP) Analysis

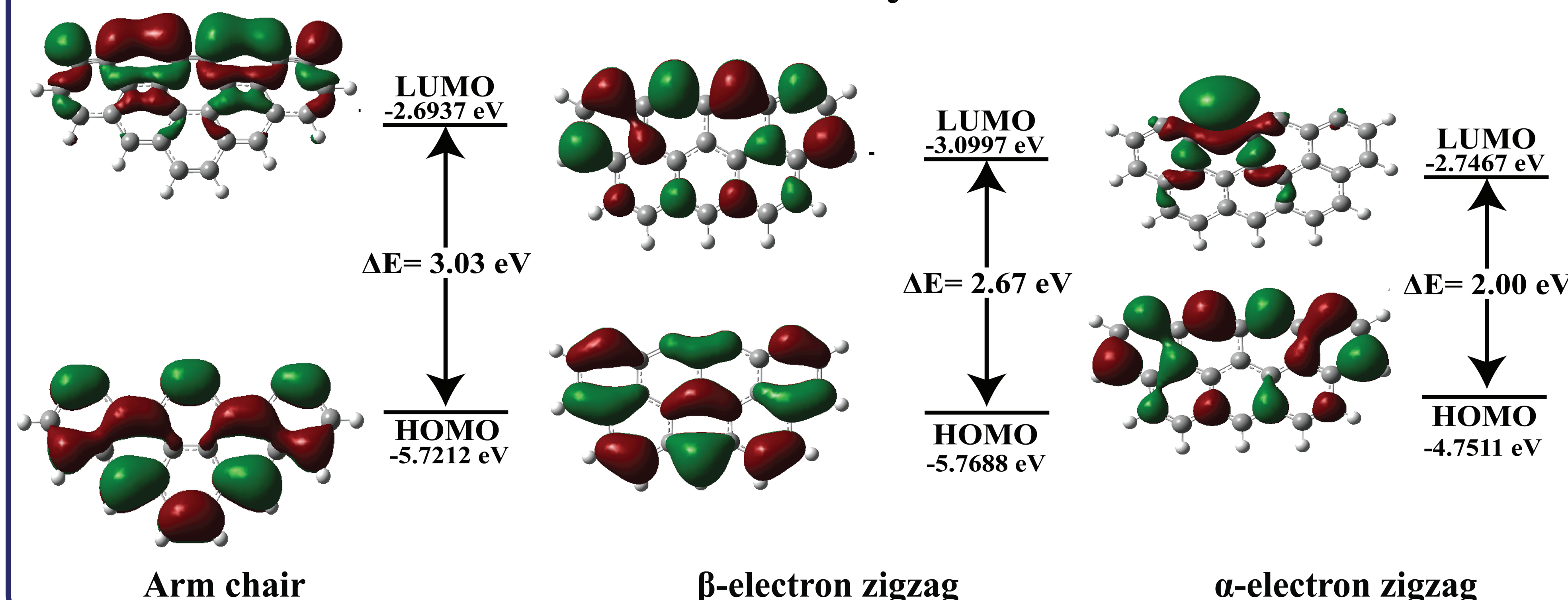


armchair configuration

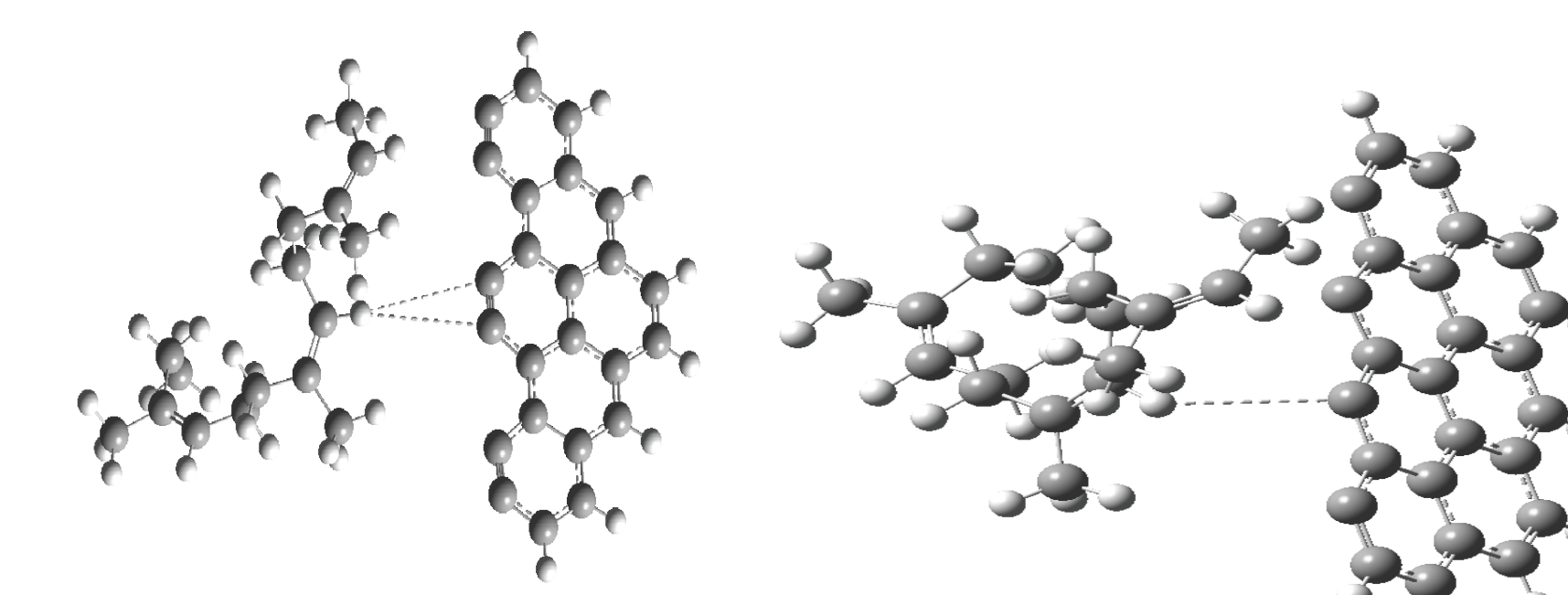


zig-zig configuration

Frontier Molecular Orbital Analysis



Adsorption Analysis



armchair and
cis 1,4-isoprene

zigzag
cis 1,4-isoprene

cis 1,4-isoprene	
Edge type	Adsorption Energy (kcal.mol ⁻¹)
Armchair	-0.47
Zig-zag	-5.33

Conclusion

The zigzag edge configuration exhibits higher electronic reactivity than the armchair edge. Stronger adsorption of 1,4-cis-isoprene on zigzag edges demonstrates superior interaction capacity.

Reference

1. Weber et al. (2018). Properties of biochar. Fuel, 217, 240–261. <https://doi.org/10.1016/j.fuel.2017.12.054>
2. Navak et al. (2009). Characterization of designer biochar produced at different temperatures and their effects on a loamy sand. Annals of Environment Science, 3, 195–206.

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Relevance to SDGs

