## Influence of sumanene modifications with boron and nitrogen atoms to its hydrogen adsorption properties

Stevan Armaković<sup>1</sup>, Sanja J. Armaković<sup>2,\*</sup>, Svetlana Pelemiš<sup>3</sup>, Dragoljub Mirjanić<sup>4,5</sup>

- <sup>1</sup> University of Novi Sad, Faculty of Sciences, Department of Physics, Trg Dositeja Obradovića 4, 21000, Novi Sad, Serbia,
  - <sup>2</sup> University of Novi Sad, Faculty of Sciences, Department of Chemistry, Biochemistry and Environmental Protection, Trg Dositeja Obradovića 3, 21000, Novi Sad, Serbia,
  - <sup>3</sup> University of East Sarajevo, Faculty of Technology, Zvornik, Karakaj bb, 75400 Zvornik, Republic of Srpska, Bosnia and Herzegovina
- <sup>4</sup> University of Banja Luka, Medical Faculty, 78000 Banja Luka, Republic of Srpska, Bosnia and Herzegovina

<sup>5</sup>Academy of Sciences and Arts of the Republic of Srpska, Trg srpskih vladara 2, 78000 Banja Luka, Republic of Srpska, Bosnia and Herzegovina

## \* Corresponding Author: Sanja J. Armaković,

Telephone: +381 21 485 2754

E-mail: sanja.armakovic@dh.uns.ac.rs

## Supplementary Information

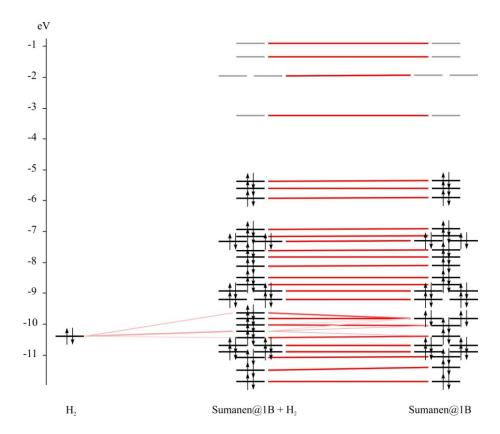


Figure S1. Fragment analysis of system consisting of sumanene derivative

modified with one boron atom and  $\mathrm{H}_2$ 

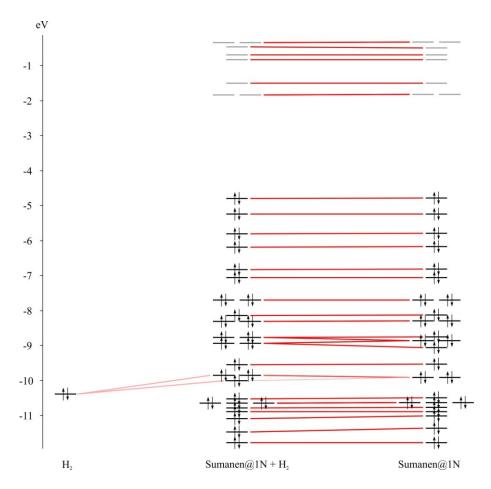


Figure S2. Fragment analysis of system consisting of sumanene derivative modified with one nitrogen atom and  $H_2$ 

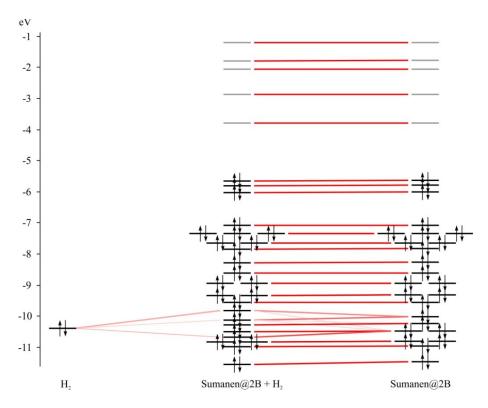


Figure S3. Fragment analysis of system consisting of sumanene derivative modified with two boron atoms and  $H_2$ 

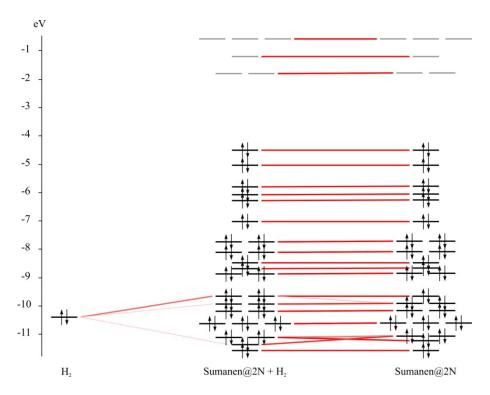


Figure S4. Fragment analysis of system consisting of sumanene derivative modified with two nitrogen atoms and  $H_2$