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A theoretical survey on the chlorine dioxide (ClO_2) and its decomposed species detection by the AlN nanotube in presence of environmental gases

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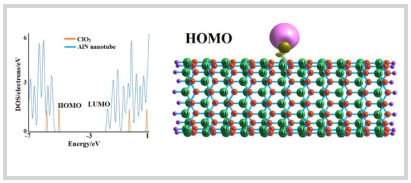
Abstract

The adsorption of N_2, O_2, H_2O, hydrogen chloride (HCl), Cl_2, hypochlorous acid (HClO), and ClO_2 gases was explored onto an AlN nanotube (AlNNT) through density functional theory computations. As N_2, O_2, H_2O, HCl, Cl_2, and HClO approach the AlNNT, their adsorption releases 7.1, 12.6, 22.3, 26.5, 30.2, and 41.2 kJ/mol of energy, respectively, indicating a physisorption. In addition, the electronic properties of the nanotube do not change significantly. As chlorine dioxide (ClO_2) approaches the AlNNT, its adsorption releases 97.4 kJ/mol of energy. Electronic analysis showed that the AlNNT HOMO–LUMO gap reduces from 4.10 to 2.80 eV (~ – 31.7%) by ClO_2 adsorption and the electrical conductivity increases significantly. Therefore, the AlNNT can generate electrical signals when the ClO_2 molecules approach, being a hopeful sensor. It was found that this nanotube can selectively detect ClO_2 gas among the mentioned molecules. The recovery time for the AlNNT was computed to be 8.0 s for ClO_2 desorption, representing a short recovery time.

Graphical abstract



References

1. Gharibzadeh F, Vessally E, Edjlali L, Es'haghi M, Mohammadi R (2020) Iran J Chem Chem Eng 39:51–62. https://doi.org/10.30492/ijcce.2020.106867.3568

2. Vessally E, Babazadeh M, Alipour F, Hosseinian A, Kheirollahi Nezhad PD (2021) Iran J Chem Chem Eng 40:691–703. https://doi.org/10.30492/ijcce.2020.122123.3987

3. Ahmadi S, Hosseinian A, Kheirollahi Nezhad PD, Monfared A, Vessally E (2019) Iran J Chem Chem Eng 38:1–19. https://doi.org/10.30492/ijcce.2019.33786

4. Vessally E, Mohammadi S, Abdoli M, Hosseinian A, Ojaghloo P (2020) Iran J Chem Chem Eng 39:11–19. https://doi.org/10.30492/ijcce.2019.36288

5. Vessally E, Farajzadeh P, Najafi E (2021) Iran J Chem Chem Eng 40:1001–1011. https://doi.org/10.30492/ijcce.2021.141635.4498

6. Ma X, Kexin Z, Yonggang W, Ebadi AG, Toughani M (2021) Iran J Chem Chem Eng. https://doi.org/10.30492/IJCCE.2021.529010.4694

7. Hashemzadeh B, Edjlali L, Kheirollahi Nezhad PD, Vessally E (2021) Chem Rev Lett. https://doi.org/10.22034/crl.2020.187273.1087

8. Salehi N, Vessally E, Edjlali L, Alkorta I, Eshaghi M (2000) Chem Rev Lett 3:207–217. https://doi.org/10.22034/crl.2020.230543.1056

9. Sreerama L, Vessally E, Behmagham F (2020) J Chem Lett 1:9–18. https://doi.org/10.22034/jchemlett.2020.106645

10. Kumar S (2008) ALD growth of a novel mixed-phase barrier for seedless copper electroplating applications. State University of New York, Albany

11. Majedi S, Sreerama L, Vessally E, Behmagham F (2020) J Chem Lett 1:25–31. https://doi.org/10.22034/jchemlett.2020.107760

12. Moradi O, Zare K, Monajjemi M, Yari M, Aghaie H (2010) Fullerenes Nanotub Carbon Nanostruct 18:285

13. Moradi O, Zare K (2011) Fullerenes Nanotub Carbon Nanostruct 19:628

14. Ahmadi A, Kamfiroozi M, Beheshtian J, Hadipour NL (2011) Struct Chem 22:1261–1265

15. Baei MT, Peyghan AA, Bagheri Z (2012) Chin Chem Lett 23:965–968

16. Baei MT, Peyghan AA, Bagheri, Z (2013) Struct Chem 24:1099–1103

17. Beheshtian J, Peyghan AA, Bagheri Z, Tabar MB (2013) Struct Chem 25:1–7

18. Moradi M, Peyghan AA, Bagheri Z, Kamfiroozi M (2012) J Mol Model 18:3535–3540

19. Wang Z, Lei Q, Wang Z, Yuan H, Cao L, Qin N, Liu J (2020) Chem Eng J 395:125180. Lausanne, Switzerland. https://doi.org/10.1016/j.cej.2020.125180

20. Peyghan AA, Baei MT, Moghimi M, Hashemian S (2012) Comput Theor Chem 997:63–69

21. Koao LF, Hone FG, Dejene FB (2020) J Nanostruct Chem 10:1

22. Aragaw BA (2020) J Nanostruct Chem 10:9

23. Malinga NN, Jarvis ALL (2020) J Nanostruct Chem 10:55

24. Peyghan AA, Noei M (2014) Physica B: Condensed Matter 432:105–110

25. Peyghan AA, Soleymanabadi H (2015) Current Science 108:1910–1914

26. Robati D, Bagheriyan S, Rajabi M, Moradi O, Peyghan AA

(2016) Physica E 83:1–6

27. Zhang X, Tang Y, Zhang F, Lee C (2016) Adv Energ Mater 6(11):1502588. https://doi.org/10.1002/aenm.201502588

28. Ji B, Zhang F, Song X, Tang Y (2017) Adv Mater (Weinheim) 29(19):1700519. https://doi.org/10.1002/adma.201700519

29. Beheshtian J, Baei MT, Peyghan AA, Bagheri Z (2013) J Mol Model 19:943

30. He C, Wang J, Fu L, Zhao C, Huo J (2021) Chin Chem Lett. https://doi.org/10.1016/j.cclet.2021.09.009

31. Jiang L, Wang Y, Wang X, Ning F, Wen S, Zhou Y, Zhou F (2021) Appl Sci Manuf 147:106461. https://doi.org/10.1016/j.compositesa.2021.106461

32. Hu L, Huang X, Zhang S, Chen X, Dong X, Jin H, Jiang Z (2021) Mater Electron 32(19):23728. https://doi.org/10.1007/s10854-021-06464-7

33. Li Y, Macdonald DD, Yang J, Qiu J, Wang S (2020) Corros Sci 163:108280. https://doi.org/10.1016/j.corsci.2019.108280

34. Xie Y, Meng X, Mao D, Qin Z, Wan L, Huang Y (2021) ACS Appl Mater Interfaces 13(27):32161–32174. https://doi.org/10.1021/acsami.1c07148

35. Rezaei A, Ghiasi R, Marjani A (2020) J Nanostruct Chem 10:179

36. Najafi F (2020) J Nanostruct Chem 10:227

37. Foroutan M, Fatemi SJ, Fatemi SM (2020) J Nanostruct

Chem 10:265

38. Rodrigues BS, Almeida VA, Claudino CH, Ponce-de-Leon C, Bavykin DV, Souza JS (2020) J Nanostruct Chem 10:363

39. Baei MT (2012) Monatsh Chem 143:545

40. Mirzaei M, Mirzaei M (2011) Monatsh Chem 142:115

41. Noei M, Salari AA, Ahmadaghaei N, Bagheri Z, Peyghan AA (2013) C R Chim 16:985

42. Samadizadeh M, Rastegar SF, Peyghan AA (2015) Phys E 69:75

43. Mohammadi R, Hosseinian A, Khosroshahi ES, Edjlali L, Vessally E (2018) Phys E 98:53

44. Baei MT, Peyghan AA, Bagheri Z (2013) Superlattices Microstruct 53:9

45. Hu M, Wang Y, Yan Z, Zhao G, Zhao Y, Xia L, Zhuang X (2021) Mater Energ Sustain 9(24):14093–14100. https://doi.org/10.1039/D1TA01505B

46. Ahmadi A, Hadipour NL, Kamfiroozi M, Bagheri Z (2012) Sens Actuators B 161:1025

47. Ahmadi Peyghan A, Omidvar A, Hadipour NL, Bagheri Z, Kamfiroozi M (2012) Phys E 44:1357

48. Fu Y, Chen H, Guo R, Huang Y, Toroghinejad MR (2021) J Alloy Compd 888:161507. https://doi.org/10.1016/j.jallcom.2021.161507

49. Yang M, Kong Q, Feng W, Yao W, Wang Q (2021) Appl Surf Sci 569:150984. https://doi.org/10.1016/j.apsusc.2021.150984

50. Zhang C, Liu X, Liu C, Luo X (2021) J Kansas Entomol Soc. https://doi.org/10.2317/0022-8567-93.4.267

51. Yan Y, Feng L, Shi M, Cui C, Liu Y (2020) Food Chem 306:125589. https://doi.org/10.1016/j.foodchem.2019.125589

52. Shi M, Wang F, Lan P, Zhang Y, Zhang M, Yan Y, Liu Y (2021) Food Sci Technol 138:110677. https://doi.org/10.1016/j.lwt.2020.110677

53. Baei MT, Peyghan AA, Bagheri Z, Tabar MB (2012) Phys Lett A 377:107

54. Priya DD, Khan MMR, Roopan SM (2020) J Nanostruct Chem 10:289

55. Rita A, Sivakumar A, Sahaya Jude-Dhas S, Martin-Britto-Dhas SA (2020) J Nanostruct Chem 10:309

56. González-Ballesteros N, Rodríguez-Argüelles MC, Lastra-Valdor M, González-Mediero G, Rey-Cao S, Grimaldi M, Cavazza A, Bigi F (2020) J Nanostruct Chem 10:317

57. Kozlovskiy A, Zdorovets M, Kenzhina I, Berguzinov A, Tishkevich D, Zubar T, Trukhanov A (2020) J Nanostruct Chem 10:331

58. Rehman Y, Copet C, Morlando A, Huang XF, Konstantinov K (2020) J Nanostruct Chem 10:347

59. Moradi O, Zare K (2013) Fullerenes Nanotub Carbon Nanostruct 21:449

60. Adhikari K, Ray A (2011) Phys Lett A 375:1817

61. Zhao G, Li X, Huang M, Zhen Z, Zhong Y, Chen Q, Zhao X, He Y, Hu R, Yang T (2017) Chem Soc Rev 46:4417

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