

HU-ACE NEWS LETTER

Advanced Core for Energetics, Hiroshima University

Vol. 79
2023.7

Activities of the Core

- | | |
|-----------------|---|
| July. 3-4, 2023 | The 7th International Symposium on Fuels and Energy (ISFE2023) (organized). |
| July. 8, 2023 | The Higashi-Hiroshima Energy Eco Seminar 2nd "Using the Energy of Grass and Trees - Biomass" (organized). |
| July. 13, 2023 | The 81th HU-ACE Steering Committee Meeting.
The 133th Mechanical Systems Seminar (co-organized). |
| July. 15, 2023 | The Higashi-Hiroshima Energy Eco Seminar 3rd "Energy Saving Air Conditioning with Heat from the Earth: Geothermal Heat"(organized). |
| July. 25, 2023 | The 108th Hiroshima University Biomass Evening Seminar (co-organized). |
| July. 29, 2023 | Kids Energy Symposium 2023 (co-organized). |

ISFE2023 was held in hybrid style

The 7th International Symposium on Fuels and Energy (ISFE2023), organized by the Advanced Core for Energetics, Hiroshima University (HU-ACE), was successfully held on July 3 and 4 at the Higashi-Hiroshima Arts & Culture Hall "KURARA". We had 9 keynote lectures, 25 oral presentations and 26 poster presentations. In total, 67 participants from 8 countries attended this symposium. The keynote lectures on wind, solar and nuclear power (Day 1), and those on biomass utilization in Thailand, Indonesia and Malaysia (Day 2) were each followed by general discussions with the keynote speakers. We deepened discussions on the "Hiroshima Scenario to realize a decarbonized society," which has been developed by the past ISFEs, and to promote international information exchange. We were able to hold the first face-to-face ISFE in four years. While "KURARA" was used as the main venue, access environment via Zoom was provided to online participants. The hybrid style connected onsite and online participants for lively discussions and exchanges of opinions. We would like to thank all participants and all those who supported in the preparation and operation of ISFE2023.



Related events

The next 8th International Symposium on Fuels and Energy (ISFE2024) is scheduled on July 1-2, 2024. Details will be announced later.

Obituary: Dr. Koichi Yamada, who was our advisor, passed away due to his disease on Jul. 6. We will continue our activities including Hiroshima Scenario with his advice in our mind.



Research consultation and joint research are welcome.

Issued by Advanced Core for Energetics, Hiroshima University
HU-ACE Secretariat, URA Division, Office of Research and Academia-Government-Community
Collaboration, Hiroshima University 1-3-2 Kagamiyama, Higashi-Hiroshima, 739-8511 Japan
E-mail: hu-ace-info@ml.hiroshima-u.ac.jp, tel:+81-82-424-4425, URL: <https://hu-ace.hiroshima-u.ac.jp/en/>

Member Introduction

MENGLI ZHANG

Assistant Professor, Mechanical Engineering Program, Hiroshima University

Research Field : Mechanical Physics, Material

Keyword : Carbon nanotubes, gas sensors and molecular adsorption mechanisms.



Abstract

Background

In 1991, Japanese scientist Iijima observed multi-walled carbon nanotubes (MWCNTs) using a transmission electron microscope, and since then, carbon nanotubes (CNTs) have attracted significant attention as a potential material for gas sensors due to their unique chemical and physical properties. Compared to traditional gas sensors, CNT gas sensors show higher sensitivity, faster response time, and a wider range of detectable concentrations. However, carbon nanotube gas sensors for measuring the common organic contaminants that are present in our environment still lack study.

Method

The fitting model of the adsorption isotherm and the sensing parameters of sensitivity, response and recovery time, and reproducibility of the gas sensor based on the Langmuir isotherm model and the Type VI isotherm model were examined. The results showed that the Langmuir adsorption model fits well with the experimental data for the polar molecules. While the adsorption behavior of non-polar gas molecules can be fit by the Type VI isotherm model. Based on the model results two hypotheses were proposed for the adsorption mechanism of these molecules: a line parallel structure, in which the molecules are arranged in the same plane parallel to the graphene, and a sandwich structure, in which the second layer of molecules is located on top of the first layer that has been adsorbed onto the surface of graphene. To prove these hypotheses, Gaussian 16 software was used to calculate the total energy of each possible structure. It's determined that the structure with the lowest adsorption energy consumption is the one most likely to be adopted by the molecules due to its chemical stability.

Results

The results showed that for benzene molecules, the lowest total energy was 9.87 fJ in a sandwich structure with a distance of 60 pm between Benzene molecules and a distance of 43.56 pm between two layers of graphene. For methanol molecules, the lowest total energy was 9.00 fJ in a parallel structure with a distance of 220 pm between methanol molecules and a distance of 284.6 pm between two layers of graphene. This indicates that non-polar molecules are adsorbed by graphene in a sandwich structure, with the second layer of molecules located on top of one another, while polar molecules showed one-layer adsorption in a parallel structure.

Reference

M.L. ZHANG, et al., Chem. Phy. Lett. 798 (2022)139596

