

## Prediction of Chemical Safety with Neural Network

Kazutoshi TANABE,<sup>1</sup> Norihito OHMORI,<sup>1</sup> Shuichiro ONO,<sup>1</sup>

Takahiro SUZUKI,<sup>2</sup> Takatoshi MATSUMOTO,<sup>3</sup> and Hiroyuki UESAKA<sup>4</sup>

<sup>1</sup>Department of Management Information Science, Chiba Institute of Technology,  
Tsudanuma 2-17-1, Narashino-shi, Chiba 275-0016, Japan

<sup>2</sup>Department of Economics, Toyo University, Hakusan 5-28-20, Bunkyo-ku, Tokyo 112-8606, Japan

<sup>3</sup>Institute of Multidisciplinary Research for Advanced Materials, Tohoku University,  
Katahira 2-1-1, Aoba-ku, Sendai-shi, Miyagi 980-8577, Japan

<sup>4</sup>Department of Regional Science, Toyama University of International Studies,  
Higashikuromaki 65-1, Ohyama-cho, Kamishinkawa-gun, Toyama 930-1292, Japan

Tel/FAX: 047-478-0344 e-mail: [tanabe@pf.it-chiba.ac.jp](mailto:tanabe@pf.it-chiba.ac.jp)

A neural network was applied to the prediction of the carcinogenicity of many organic compounds. Data of the Challenge contest were used and the performance of our method was compared with those of contestants. Three groups of descriptors, Dragon, tReymers, and Helma were tested. The classification test using 18 tReymers descriptors showed a correct classification rate close to 90%, higher than any of the contestants.

## Sustainable Amelioration of Semi-arid Arable Land with Bio-remediation Technology

Yuuki Yazawa, Takayoshi Kobayashi, Parida Yamada, Tatsuaki Yamaguchi

Faculty of Engineering, Chiba Institute of Technology

2-17-1 Tsudanuma, Narashino, Chiba 275-0016, Japan

Tel: 047-478-0424, Fax: 047-478-0439, [yyazawa@pf.it-chiba.ac.jp](mailto:yyazawa@pf.it-chiba.ac.jp)

As focused on the previous COP and WSSD meeting, the ratification statement and concrete countermeasure for the Kyoto protocol (strategies to reduce emissions of greenhouse gases) makes urgent necessity all over the world. Especially, the establishment of the essential technology of "sustainable development" is required for this purpose. In this study, the bio-remediation technology for semi-arid arable land was investigated to meet the requirement

## Environmentally Benign Removal of Pollutant Oxyanions by Fe Adsorption Center in Functionalized Mesoporous Silica

Toshiyuki Yokoi<sup>1</sup>, Hideaki Yoshitake<sup>2</sup> and Takashi Tatsumi<sup>1</sup>

<sup>1</sup> Division of Materials Science and Chemical Engineering, Graduate school of Engineering, Yokohama National University, 79-5 Tokiwadai, Hodogaya-ku, Yokohama 240-8501, Japan

Tel & Fax: +81-45-339-3941, E-mail: [d02sa104@ynu.ac.jp](mailto:d02sa104@ynu.ac.jp)

<sup>2</sup> Graduate School of Environment and Information Sciences, Yokohama National University, 79-7 Tokiwadai, Hodogaya-ku, Yokohama 240-8501, Japan

We have synthesized the specific molecular adsorption sites on the pore wall surface in MCM-41 by means of fixation of ethylenediamine group followed by cationization with Fe<sup>3+</sup>. The iron-anchored surface sites result in fast and selective adsorptions of pollutant oxyanions, such as arsenate, chromate, selenate and molybdate.

**PROMOTING SUSTAINABILITY IN THE WORKPLACE THROUGH THE USE OF  
EMPLOYEE QUESTIONNAIRE**

MARIA ANN MAH, CWBIOS INC., 113 339 50<sup>TH</sup> AVE., S.E.

CALGARY, ALBERTA, CANADA T2G 2B3

TEL: 403-255-3788, FAX: 403-255-3788, E-MAIL: NINE21@TELUS.NET

Behavior in the workplace is a complex experience of stress associated with actions, decisions, information and emotion. These influence employees' environmental, economical, and social preferences, which have important implications for developmental efforts and projects. Although sustainability has been focused on design, development, and implementation of work processes and materials (1), knowledge on the intervention of human behavior and its effects on sustainability have been at its infancy (2). Examining human behaviors will promote the coexistence between employees and the creation of sustainable workplace.

**GREEN CHEMISTRY EDUCATION AT THE  
AMERICAN CHEMICAL SOCIETY**

Mary M. Kirchhoff, Green Chemistry Institute, 1155 Sixteenth Street, N.W., Othmer 321, Washington, DC, 20036,  
202-872-4562 (P), 202-872-6206 (F), [m\\_kirchhoff@acs.org](mailto:m_kirchhoff@acs.org)

Dennis L. Hjeresen, Green Chemistry Institute, 1155 Sixteenth Street, N.W., Othmer 322, Washington, DC, 20036,  
202-872-4078 (P), 202-872-6206 (F), [d\\_hjeresen@acs.org](mailto:d_hjeresen@acs.org)

The American Chemical Society's (ACS) commitment to green chemistry was strengthened by its alliance with the Green Chemistry Institute in January 2001. ACS recognizes that one of the best ways to promote the adoption of green chemistry across the chemical enterprise is through education. Consequently ACS, with support from the U.S. Environmental Protection Agency, has been active in the development of educational materials and programs for a variety of audiences.

**IMPROVED PERFORMANCE OF OXYGEN ELECTRODE IN CELLS BY COBALT  
COMPLEXES**

BAOQING SHENTU, KENICHI OYAIZU, AND HIROYUKI NISHIDE

Department of Applied Chemistry, Waseda University, Tokyo 169-8555, Japan

+81-3-3200-2669, FAX: +81-3-3209-5522, E-MAIL: SHENTU@SUOU.WASEDA.JP - [NISHIDE@WASEDA.JP](mailto:NISHIDE@WASEDA.JP)

We report, for the first time, that cobalt complexes, which reversibly bind and release oxygen, functioned as oxygen carriers or accumulating media for an electrode to enhance the diffusion-limited current for the oxygen

reduction. It was found that a larger reduction current was obtained when an electrode was modified with the oxygen carrier based on the rapid release of oxygen from the carrier, which could practically be employed in superior air battery and fuel cell.