

業績目録(宮本明)

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宮本 明教授業績目録

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東北大学史料館
(著作目録第 1211 号)



宮本 明教授略歴

生年月日	1947年5月3日
本籍地	三重県
職名	教授
所属	未来科学技術共同研究センター 工学研究科（兼任）

最終学歴

1970年3月	東北大学工学部応用化学科卒業
1972年3月	東北大学大学院工学研究科化学工学専攻修士課程修了
1975年3月	東北大学大学院工学研究科化学工学専攻博士課程修了

職歴

1975年4月	名古屋大学工学部助手
1985年5月	京都大学工学部助教授
1992年4月	東北大学工学部教授
1997年4月	東北大学大学院工学研究科教授 現在に至る
2002年4月	東北大学未来科学技術共同研究センター教授（現在に至る）
2008年4月	東北大学 デイスティングイッシュュトプロフェッサー任命（2010.3まで）
2009年4月	東北大学未来科学技術共同研究センター長就任（2011.3まで）
2012年3月	東北大学を定年退職

< 客員・非常勤講師歴 >

東京工業大学工業材料研究所客員教授（1994.4 - 1995.3）
通商産業省工業技術院物質工学工業技術研究所流動研究員（1995.1 - 1995.2）
科学技術庁金属材料技術研究所客員研究官（1997.4 - 2004.3）
一関工業高等専門学校非常勤講師（1997.4 - 1997.9）
九州大学工学部非常勤講師（1998.4 - 1999.3）

豊橋技術科学大学非常勤講師 (1999. 2)
科学技術庁無機材質研究所客員研究官 (1999. 4 - 2001. 3)
岩手大学工学部非常勤講師 (1997. 7 - 現在)

学 位

1975年 3月 工学博士 (東北大学)

受 賞

Hindustan Platinum Award
Computer modelling studies to locate porphyrin complexes inside microporous materials
A. Chatterjee, A. K. Chandra, S. Pal, R. Vetrivel, M. Kubo, and A. Miyamoto
Catalysis Society of INDIA (1994).

マテリアルライフ学会論文賞
計算化学手法によるゼオライトの熱劣化過程の検討
近江靖則, 宮本明, 佐野庸治
(2003年9月25日)

日本コンピュータ化学会2007年度論文賞
「不規則性多孔体微細構造最適化のための三次元多孔質シミュレータ POCO2の開発と応用」
古山通久, 扇谷恵, 服部達哉, 福長博, 鈴木愛, Riadh Sahnoun, 坪井秀行, 畠山望, 遠藤明,
高羽洋充, 久保百司, Carlos A. Del Carpio, 宮本明
(2008年5月22日)

日本コンピュータ化学会2008年度学会賞
宮本明
(2009年5月21日)

学会等における活動 (役職等)

○日本化学会

日本化学会幹事 (1981. 4 -1982. 3)
日本化学会代議員 (1991. 4 - 1992. 3)
日本化学会編集委員 (1992. 4 -1994. 3)
日本化学会情報化学部会副部会長 (1994. 4 - 1996. 3)
日本化学会編集委員 (1996. 4 -1998. 3)
日本化学会情報化学部会幹事 (1996. 4 - 1998. 3)
日本化学会情報化学部会監査 (1998. 4 - 1999. 3)

○化学工学会

化学工学会国際交流委員会委員 (1993.4 - 1995.3)
化学工学会出版委員会委員 (1993.4 - 1995.3)
化学工学会研究部門委員会委員 (1994.4 - 1995.3)
化学工学会分子シミュレーション工学研究会代表 (1995.4 - 2002.3)
化学工学会システム・情報・シミュレーション部会副部会長 (2002.4-)
化学工学会反応工学部会触媒反応工学分科会幹事 (2002.4-)
化学工学会代議員 (2004.4-2008.3)

○触媒学会

- 触媒学会企画委員 (1991.1 - 1992.12)
- 触媒学会編集委員 (1991.1 - 1991.12)
- 触媒学会「コンピュータ利用研究会」世話人代表 (1993.1 - 1995.12)
- 触媒学会幹事 (1995.1 - 1996.12)
- 触媒学会「コンピュータ利用研究会」事務局長 (1996.1 - 1998.12)
- 触媒学会「コンピュータ利用研究会」世話人代表 (1999.1 - 2001.12)
- 触媒学会「コンピュータ利用研究会」事務局長 (2002.1 - 現在)
- 触媒学会「天然ガス高度利用触媒研究会」世話人 (2000.1 - 2004.3)
- 触媒学会「マイクロリアクター研究会」世話人 (2002.1 - 2004.3)
- 触媒学会関東地区幹事 (2005.1 - 2006.12)
- 触媒学会関東地区代議員 (2006.1-2007.12)

○日本表面科学会

- 日本表面科学会編集委員 (1983.6 - 1987.5)
- 日本表面科学会企画委員 (1990.6 - 1991.5)
- 日本表面科学会評議員 (1991.6 - 1993.5)
- 日本表面科学会東北支部長 (1993.6 - 1996.5)
- 日本表面科学会理事 (1993.6 - 1997.5)
- 日本表面科学会評議員 (1997.6 - 2008.5)
- 日本表面科学会講演大会委員会委員 (1995.6-2001.5)
- 日本表面科学会東北支部監査 (1996.6-1998.5)
- 日本表面科学会東北支部企画幹事 (1998.6-2007.5)
- 日本表面科学会出版委員会委員 (2000.6 -2002.5)
- 日本表面科学会講演大会委員会委員 (2000.6-2002.5)
- 日本表面科学会会員増強委員会委員 (2001.6-2002.5)

○ゼオライト学会

- 理事 (1995.1-1996.12)

○日本コンピュータ学会

- 理事 (2002.1- 現在)

○NEDO

- NEDO フロン分解技術調査研究推進委員会委員 (1995.11-1996.3)
- NEDO ハード新材料素子化技術調査委員会委員 (1997.4-1998.3)
- NEDO 計算機材料設計の調査研究委員会委員 (1997.4-1999.3)

○日本トライボロジー学会

- 日本トライボロジー学会トライボロジー会議2002実行委員会委員 (2002.1-2002.12)
- 日本トライボロジー学会分子シミュレーションのトライボロジーへの応用に関する研究会委員 (2005.4-2006.3)

○その他

- 近畿化学協会コンピュータ化学部会幹事 (1991.4 - 1993.3)
- 表面機能材料研究会幹事 (1991.4 - 1992.3)
- 通商産業省産業技術審議会専門委員 (1998.2-2000.2)
- 財団法人化学技術戦略推進機構調査委員 (2000.3-2001.3)

青葉工業会常任理事 (2001.4-2003.3)

財団法人大阪科学技術センター附属ニューマテリアルセンター「合金系水素貯蔵材料の耐久性研究」評価解析ワーキンググループ委員 (2003.8-2004.3)

財団法人大阪科学技術センター附属ニューマテリアルセンター「合金系水素貯蔵材料の耐久性研究」評価解析ワーキンググループ委員 (2006.1-2008.3)

○国際会議組織委員等

[1992]

7th International Symposium on Relations between Homogeneous and Heterogeneous Catalysis Postsymposium of VII-SHHC in Kyoto
(Kyoto, Japan, May 23-24, 1992)
Member of Organizing Committee

The Second International Conference & Exhibition on Computer Applications to Materials and Molecular Science and Engineering
(Yokohama, Japan, September 22-25, 1992)
Member of Executive Committee & Scientific Chairman of Catalyst Session

[1993]

Sendai Meeting on New Trends in Zeolite Science
(Sendai, Japan, August 27, 1993)
Organizer

[1994]

International Workshop on Catalytic Combustion
(Tokyo, Japan, April 17-20, 1994)
Member of Organizing Committee

Second Tokyo Conference on Advanced Catalytic Science and Technology
(Tokyo, Japan, August 21-26, 1994)
Member of Organizing Committee

Post Conference Symposium of TOCAT-2
Impacts of Computers on Catalyst Research and Development
(Sendai, Japan, August 28-30, 1994)
General Secretary

[1997]

International Symposium on Zeolites and Microporous Crystals '97
(Tokyo, Japan, August 24-27, 1997)
Member of Organizing Committee

International Workshop on Hard Electronics
(Tsukuba, Japan, February 17-18, 1997)
Member of Organizing Committee

[1998]

9th International Conference on Modern Materials & Technologies

(Florence, Italy, June 14-19, 1998)

Member of Advisory Committees of Topical Symposium I

Fifth Liblice Conference on the Statistical Mechanics of Liquids

(Zelezna Ruda, Czech Republic, June 7-12, 1998)

Member of Scientific Advisory Committee

International Workshop on Hard Electronics'98

(Tsukuba, Japan, February 3-4, 1998)

Member of Organizing Committee

Post Conference Symposium of TOCAT-3

Impacts of Computers on Catalyst Research and Development 2

(Kyoto, Japan, July 26-28, 1998)

Secretariat

[1999]

International Symposium on Recent Advances in Density Functional Theory

(Sendai, Japan, April 19, 1999)

Chairman

Indo-Japan Workshop on Materials Design by Computer Simulation

(Sendai, Japan, August 24, 1999)

Chairman

[2000]

International Symposium on Zeolites and Microporous Crystals 2000

(Sendai, Japan, August 6-9, 2000)

Chairman

International Symposium on Research and Education in the 21st Century:

(Sendai, Japan, August 18-25, 2000)

Member of Organizing Committee

International Symposium on Molecular Design of Catalysts

(Sendai, Japan, August 22, 2000)

Chairman

Symposium on Synthesis of Ecological High Quality Transportation Fuels

(Sendai, Japan, August 23, 2000)

Member of Organizing Committee

Tribochemistry Tsukuba 2000

(Tsukuba, Japan, October 27, 2000)

Vice-Chairman

[2001]

Bangkok International Conference on Heterogeneous Catalysis

(Bangkok, Thailand, January 7-9, 2001)

Member of Organizing Committee

SPIE's International Symposium on Integrated Optoelectronic Devices (Optoelectronics 2001),
"Combinatorial and Composition Spread Techniques in Materials and Device Development II"
Session

(San Jose, USA, January 19-26, 2001)

Member of Program Committee

Ninth International Conference on Properties and Phase Equilibria for Product and Process
Design

(Kurashiki, Japan, May 20 - May 25, 2001)

Member of Local Organizing Committee

[2002]

2nd International Symposium on Synthesis of Ecological High Quality Transportation Fuels

(Osaka, Japan, January 22-23, 2002)

Member of Organizing Committee

The Fourth Tokyo Conference on Advanced Catalytic Science and Technology

(Tokyo, Japan, July 14-19, 2002)

Member of Organizing Committee

The Second US-Japan Workshop on Combinatorial Materials Science and Technology

(Colorado, USA, August 9-11, 2002)

Member of Organizing Committee

[2003]

1st International Symposium of Theoretical Methods for "Giant Molecules and Complex
System"

(Sendai, Japan, May 28, 2003)

Chairman

International Symposium on Zeolites and Microporous Crystals 2003

(Sapporo, Japan, August 3-6, 2003)

Member of Organizing Committee

[2004]

The 3rd International Conference on Computational Modeling and Simulation of Materials

(Sicily, Italy, May 29-June 5, 2004)

Member of International Advisory Committee

1st International Symposium on Combinatorial Computational Chemistry

(Sendai, Japan, August 8, 2004)

Chairman

2nd International Symposium on Combinatorial Computational Chemistry

(Sendai, Japan, November 20, 2004)

Chairman

2nd International COE Symposium for "Giant Molecules and Complex Systems"
(Sendai, Japan, November 22-23, 2004)
Member of Organizing Committee

[2005]

Tribochemistry Nara 2005
(Nara, Japan, May 26-27, 2005)
Member of Organizing Committee

5th World Congress on Oxidation Catalysis
(Sapporo, Japan, September 25-30, 2005)
Member of Organizing Committee

[2006]

International Conference of Quantum Chemistry 2006 Workshop in Sendai
- Advances in Theoretical and Spectroscopic Studies on Electron Dynamics and Related Phenomena
(Sendai, Japan, May 17-19, 2006)
Member of Organizing Committee

11th International Conference on Theoretical Aspects of Catalysis
(Berlin, Germany, June 12-15, 2006)
Member of Advisory board

International Symposium on Zeolites and Microporous Crystals 2006
(Yonago, Japan, July 30-August 2, 2006)
Member of Organizing Committee

The 6th International Meeting on Information Display and the 5th International Display Manufacturing Conference (IMID/IDMC 2006)
(Daegu, Korea, August 22-25, 2006)
Member of Technical Program Committee

[2008]

Experiment-Integrated Computational Chemistry on Multiscale Fluidics (ECCMF)
(Miyagi, Japan, January 17- January 18, 2008)
Honorary Chairman

[2009]

World Tribology Congress 2009
(Kyoto, Japan, Sept. 6-11, 2009)
Session Organizer

International Symposium on Zeolites and Microporous Crystals 2006
(Tokyo, Japan, August 3-August 7, 2009)
Member of Organizing Committee

[2010]

The Second International Symposium of Experiment-Integrated
Computational Chemietry on Multiscale Fluidics (ECCMF2)
(Miyagi, Japan, February 23-24, 2010)
Honorary Chairman

13th International Conference on Theoretical Aspects of Catalysis
(Miyagi, Japan, June 21-June25, 2010)
Honorary Chairman

○学会誌の編集者、委員等

"Catalysis Today" 誌 Editorial Advisory Board (編集顧問委員)
(1993.4 – 2000.3)

"Applied Catalysis" 誌 News Brief Correspondents (ニュース、ブリーフ担当委員)
(1989)

"Bulletin of Chemical Society of Japan" 誌 Associate Editor (編集委員) (1992)

"Bulletin of Chemical Society of Japan" 誌 Associate Editor (編集委員) (1996)

"Catalysis Surveys from Japan" 誌 Editorial Advisory Board (編集顧問委員) (1999)

"Journal of Molecular Graphics & Modelling" 誌 誌
Editorial Advisory Board (編集顧問委員) (1998)

外部機関における活動

東京工業大学工業材料研究所 客員教授 (1994-1995)
通商産業省 工業技術院物質工学工業技術研究所 流動研究員 (1995-1995)
NEDO フロン分解技術調査研究推進委員会 委員 (1995-1996)
一関工業高等専門学校 非常勤講師 (1997-1997)
NEDO ハード新材料素子化技術調査委員会 委員 (1997-1998)
NEDO 計算機材料設計の調査研究委員会 委員 (1997-1999)
科学技術庁 金属材料技術研究所 客員研究官 (1997-2001)
岩手大学工学部 非常勤講師 (1997-2006)
通商産業省 産業技術審議会 専門委員 (1998-2000)
九州大学工学部 非常勤講師 (1998-1999)
豊橋技術科学大学 非常勤講師 (1998-1999)
科学技術庁 無機材質研究所 客員研究官 (1999-2000)
財団法人科学技術戦略推進機構 調査委員 (2000-2001)
財団法人大阪科学技術センター附属ニューマテリアルセンター
「合金系水素貯蔵材料の耐久性研究」 評価解析ワーキンググループ委員 (2003-2004)
財団法人大阪科学技術センター附属ニューマテリアルセンター
「合金系水素貯蔵材料の耐久性研究」 評価解析ワーキンググループ委員 (2006-2008)

【その他】

"Bulletin of Chemical Society of Japan" 誌 Associate Editor(編集委員)(その他)(1992-1994)

"Catalysis Today" 誌 Editorial Advisory Board(編集顧問委員)(その他)(1993-)

"Bulletin of Chemical Society of Japan" 誌 Associate Editor(編集委員)(その他)(1996-1998)

"Journal of Molecular Graphics & Modelling" 誌 Editorial Advisory Board(編集顧問委員)

(その他)(1998-)

"Catalysis Surveys from Japan" 誌 Editorial Advisory Board(編集顧問委員)(その他)(1999-)

社会における活動

日印自然科学協力事業, 「コンピュータ支援助触媒設計」,

Department of Science and Technology, Government of India, 1995-2000.

日タイ技術移転計画, 「ゼオライト触媒作用の計算機モデリング」, タイ国,

チュラロンコン大学, 1997-2000.

業 績 目 録

I. 著書・編書（共著書等含む）

○日本語著書

[1980]

1. 自動車エンジンの排気浄化
三元触媒：触媒の作用機構, (1980) 353-355.
村上雄一, 宮本明

[1981]

2. 触媒設計
5. 触媒物性試験, 槇書店, 10月(1981) 87-114.
服部忠, 丹羽幹, 宮本明

[1986]

3. 触媒講座別巻 触媒実験ハンドブック
2.2.1 反応操作－流通法－概説, 講談社サイエンティフィック, 5月(1986) 44-48.
宮本明
4. 触媒講座別巻 触媒実験ハンドブック
3.3.4A V_2O_5 触媒の表面 $V=O$ 数の決定, 講談社サイエンティフィック, 5月(1986) 187-189.
松田正徳, 宮本明
5. 触媒講座10 触媒各論
1. 酸化バナジウム触媒, 講談社サイエンティフィック, 6月(1986), 1-20.
宮本明
6. 触媒講座 4 反応機構決定法・錯体触媒
4.3 反応機構の決定, 講談社サイエンティフィック, 6月(1986) 312-342.
宮本明, 斉藤泰和

[1989]

7. 新材料開発とコンピューターケミストリー,
2.5 無機機能材料, 化学工業日報社, 11月(1989), 113-135.
宮本明, 乾智行

[1991]

8. 化学工学シンポジウムシリーズ28－機能性表面の解析と設計
20. ゼオライト様マイクロ多孔性結晶の分子動力学シミュレーション
化学工学会, 3月, (1991) 149-156.
宮本明, 久保百司, 服部敬宙, 松葉勝彦, 河村雄行, 乾智行

[1992]

9. 計算機化学工学
オーム社, 4月(1992).
荒井康彦, 宮本明, 亀山秀雄, 山口兆
10. 実験化学講座11 反応と速度
5.3 酸化物触媒－酸化還元反応, 丸善株式会社, 2月(1992).
宮本明

[1993]

11. 化学工学シンポジウムシリーズ35－超臨界流体の工学的利用と溶媒特性の分子論的解明
19. 表面吸着相における流体微細構造と動的挙動に関する分子動力学的研究
化学工学会, 2月, (1993) 113-118.
高羽洋充, 久保百司, 宮本明

[1994]

12. 化学工学シンポジウムシリーズ41－膜工学の新しい挑戦－1994
4. 無機分離膜のコンピュータ支援分子設計
化学工学会, 2月, (1994) 13-16.
高羽洋充, 片桐昌彦, 久保百司, Rajappan Vetrivel, 宮本明
13. 化学工学シンポジウムシリーズ41－膜工学の新しい挑戦－1994
35. 分子動力学法による無機膜構造ならびに分離機能の予測の可能性と限界に関するコメント
化学工学会, 2月, (1994) 140.
宮本明

[1995]

14. 触媒技術の動向と展望1995
1.3.6 コンピュータ化学：注目研究と動向, 4月(1995) 61-70.
宮本明

15. 高機能ゼオライトの合成と応用
1.6. コンピュータグラフィックス
シーエムシー社, 12月, (1995) 72-80.
久保百司, 宮本明
16. 化学工学の進歩29－触媒工学
16. コンピュータによる触媒分子論
化学工学会, 11月 (1995).
宮本明, 片桐昌彦, Ewa Broclawik, 久保百司
17. 先端材料事典
産業調査会, (1995).
宮本明

[1996]

18. 原子・分子で理解する固体表面現象
培風館, 7月, (1996).
小宮山政晴, 森誠之, 宮本明, 久保百司

[1997]

19. 高純度化技術体系 第2巻 分離技術
4-2-3-3 分子設計支援システム
フジテクノシステム, 2月, (1997) 417-420.
宮本明, 久保百司
20. 環境触媒－実際と展望－
2.4 計算機シミュレーションによる触媒設計
共立出版, 3月 (1997).
久保百司, 宮本明
21. 最近の化学工学49－膜技術の動向と将来展望
2-4 分離膜への分子シミュレーションの応用
化学工学会, (1997).
水上浩一, 高羽洋充, 近江靖則, 久保百司, 寺石和夫, Abhijit Chatterjee,
宮本明

[1999]

22. 季刊化学総説41 高次機能触媒の設計
環境触媒設計へのコンピュータ利用
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453. A Computational Chemistry Study on Friction of h-MoS₂ Part I: Mechanism of Single Sheet Lubrication [The Journal of Physical Chemistry B, 113 (2009) 16526-16536] Tasuku Onodera, Yusuke Morita, Ai Suzuki, Michihisa Koyama, Hideyuki Tsuboi, Nozomu Hatakeyama, Akira Endou, Hiromitsu Takaba, Momoji Kubo, Fabrice Dassenoy, Clotilde Minfray, Lucile Joly-Pottuz; Jean-Michel Martin, Akira Miyamoto
454. Novel Method Based on Quantum Chemistry for Calculation of Ion Induced Secondary Electron Emission Coefficient of MgO Surfaces [Japanese Journal of the Applied Physics 48 (2009) 04C145] Kazumi Serizawa, Hiroaki Onuma, Hiromi Kikuchi, Masaki Kitagaki, Itaru Yamashita, Ai Suzuki, Riadh Sahnoun, Michihisa Koyama, Hideyuki Tsuboi, Nozomu Hatakeyama, Akira Endou, Hiromitsu Takaba, Carlos A. Del Carpio, Momoji Kubo, Hiroshi Kajiyama, Akira Miyamoto
455. Comprehensive Model for Fuel Cell Exergetic Performance Which Includes Both ASR and Electronic Shorting [ECS Transactions Vol17 (2009) 139-148] M. C. Williams and A.Virkar, K. Yamaji, T. Horita, H. Yokokawa, A. Miyamoto and M. Koyama

456. Simulation of Electron Diffusion in TiO_2 Porous Structures in Dye-Sensitized Solar Cells [Japanese Journal of the Applied Physics 48 (2009) 04C166] Kei Ogiya, Chen Lv, Ai Suzuki, Riadh Sahnoun, Michihisa Koyama, Hideyuki Tsuboi, Nozomu Hatakeyama, Akira Endou, Hiromitsu Takaba, Carlos A. Del Carpio, Ramesh C. Deka, Momoji Kubo, Akira Miyamoto
457. A Graph Theoretical Approach for Assessing Bio-Macromolecular Complex Structural Stability [Journal of Molecular Modeling 15 (2009) 1349-1370] Carlos A. Del Carpio, Mihai Iulian Florea, Ai Suzuki, Hideyuki Tsuboi, Nozomu Hatakeyama, Akira Endou, Hiromitsu Takaba, Eiichiro Ichiishi, Akira Miyamoto
- [2010]
458. Host Emission from $\text{BaMgAl}_{10}\text{O}_{17}$ and $\text{SrMgAl}_{10}\text{O}_{17}$ Phosphor: Effects of Temperature and Defect Level [Journal of the Society for Information Display 18 (2010) 211-222] Hiroaki Onuma, Hiroaki Tanno, Ai Suzuki, Riadh Sahnoun, Michihisa Koyama, Hideyuki Tsuboi, Nozomu Hatakeyama, Akira Endou, Hiromitsu Takaba, Carlos A. Del Carpio, Momoji Kubo, Ramesh Chandra Deka, Hiroshi Kajiyama, Tsutae Shinoda, Akira Miyamoto
459. Influences of Film Deposition Condition on Friction of Diamond-Like Carbon Film: A Theoretical Investigation [Tribology Online, 5 (2010) 173-180] Tasuku Onodera, Takanori Kuriaki, Shandan Bai, Ryo Nagumo, Ryuji Miura, Ai Suzuki, Hideyuki Tsuboi, Nozomu Hatakeyama, Akira Endou, Hiromitsu Takaba, Momoji Kubo, Akira Miyamoto
460. Applying Ultra Accelerated Quantum Chemical Molecular Dynamics techniques for the evaluation of ligand protein interactions [Medicinal Chemistry Research, 19 (2010) 1-10] Kamlesh Kumar Sahu, Mohamed Ismael, Shah Md. Abdur Rauf, Ai Suzuki, Riadh Sahnoun, Michihisa Koyama, Hideyuki Tsuboi, Nozomu Hatakeyama, Akira Endou, Hiromitsu Takaba, Ramesh Chandra Deka, Carlos A. Del Carpio, Momoji Kubo, Akira Miyamoto
461. Tribochemical Reaction Dynamics of Molybdenum Dithiocarbamate on the Nascent Iron Surface: A Hybrid Quantum Chemical/Classical Molecular Dynamics Study [Journal of Nanoscience and Nanotechnology, 10 (2010) 2495-2502] Tasuku Onodera, Yusuke Morita, Ai Suzuki, Riadh Sahnoun, Michihisa Koyama, Hideyuki Tsuboi, Nozomu Hatakeyama, Akira Endou, Hiromitsu Takaba, Carlos A. Del Carpio, Ramesh C. Deka, Momoji Kubo, and Akira Miyamoto

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463. Quantum Chemistry Study of Surface Structure Effects on Secondary Electron Emission in MgO Protecting Layers for Plasma Displays [Japanese Journal of Applied Physics, 49 (2010) 04DJ14] Kazumi Serizawa, Hiroaki Onuma, Hiromi Kikuchi, Kazuma Suesada, Masaki Kitagaki, Itaru Yamashita, Ryuji Miura, Ai Suzuki, Hideyuki Tsuboi, Nozomu Hatakeyama, Akira Endou, Hiromitsu Takaba, Momoji Kubo, Hiroshi Kajiyama, and Akira Miyamoto
464. Modeling of Dye-Sensitized Solar Cells Based on TiO₂ Porous Electrode Structure Model [Japanese Journal of Applied Physics, 49 (2010) 04DP10] Mari Onodera, Kei Ogiya, Ai Suzuki, Hideyuki Tsuboi, Nozomu Hatakeyama, Akira Endou, Hiromitsu Takaba, Momoji Kubo, and Akira Miyamoto
465. Development of a quantum chemical molecular dynamics tribochemical simulator and its application to tribochemical reaction dynamics of lubricant additives [Modeling and Simulation in Materials Science and Engineering, 18 (2010) 034009] T. Onodera, A. Suzuki, H. Tsuboi, N. Hatakeyama, A. Endou, H. Takaba, M Kubo and A Miyamoto
466. A Metal-Organic Framework as An Electrocatalyst for Ethanol Oxidation Angew. [Chem. Int. Ed., Vol. 49, Issue 31, 5348-5351 (2010)] Lifan Yang, Shozo Kinoshita, Teppei Yamada, Seiichi Kanda, Hiroshi Kitagawa, Makoto Tokunaga, Takayoshi Ishimoto, Teppei Ogura, Ryo Nagumo, Arika Miyamoto, Michihisa Koyama
467. Chemical Degradation Mechanism of Model Compound, CF₃(CF₂)₃O(CF₂)₂OCF₂SO₃H, of PFSA Polymer by Attack of Hydroxyl Radical in PEMFCs [Journal of The Electrochemical Society, 157 (2010) B1305-B1309] Takayoshi Ishimoto, Ryo Nagumo, Teppei Ogura, Takashi Ishihara, Boyeong Kim, Akira Miyamoto and Michihisa Koyama
468. Porosity and Pt content in the catalyst layer of PEMFC: effects on diffusion and polarization characteristics [International Journal of Electrochemical Science] Ai Suzuki, Tatsuya Hattori, RyujiMiura, Hideyuki Tsuboi, Nozomu Hatakeyama, Hiromitsu Takaba, Mark C. Williams, Akira Miyamoto

469. Quantum Chemistry and QSPR Study on Relationship between Crystal Structure and Emission Wavelength of Eu^{2+} -Doped Phosphors [Journal of the Society for Information Display 18 (2010) 301-309] Hiroaki Onuma, Itaru Yamashita, Kazumi Serizawa, Hiroaki Tanno, Ai Suzuki, Hideyuki Tsuboi, Nozomu Hatakeyama, Akira Endou, Hiromitsu Takaba, Momoji Kubo, Hiroshi Kajiyama, Akira Miyamoto
470. Development of Computational Method for Analysis of Carrier Transfer in Light-Emitting Polymers [Japanese Journal of the Applied Physics 49 (2010) 04DK13] Itaru Yamashita, Kazumi Serizawa, Hiroaki Onuma, Ai Suzuki, Ryuji Miura, Hideyuki Tsuboi, Nozomu Hatakeyama, Akira Endou, Hiromitsu Takaba, Momoji Kubo, Mark C. Williams, Akira Miyamoto
471. A Theoretical Study on Initial Processes of Li-Ion Transport at the Electrolyte/Cathode Interface: A Quantum Chemical Molecular Dynamics Approach [Japanese Journal of the Applied Physics 49 (2010) 04DP11] Tomaru Ogawa, Masayuki Miyano, Yasuhiro Suzuki, Ai Suzuki, Hideyuki Tsuboi, Nozomu Hatakeyama, Akira Endou, Hiromitsu Takaba, Momoji Kubo, Akira Miyamoto
472. The Effect of R249S Carcinogenic and H168R-R249S Suppressor Mutations on p53-DNA Interaction, a Multi Scale Computational Study [Computers in Biology and Medicine 40 (2010) 498-508] Shah Md. Abdur Rauf, Mohamed Ismael, Kamlesh Kumar Sahu, Ai Suzuki, Michihisa Koyama, Hideyuki Tsuboi, Nozomu Hatakeyama, Akira Endou, Hiromitsu Takaba, Carlos A. Del Carpio, Momoji Kubo, Akira Miyamoto
473. Large-scale Quantum Chemical Molecular Dynamics Study on CO Oxidation Reaction on Precious Metal Surface [e-Journal of Surface Science and Nanotechnology 8 (2010) 272-274] Sunho Jung, Ai Suzuki, Hideyuki Tsuboi, Nozomu Hatakeyama, Akira Endou, Hiromitsu Takaba, Momoji Kubo, and Akira Miyamoto
474. An Elucidation of the Interaction Between Pt Particles and CeO_2 Surfaces Using Tight-binding Quantum Chemistry Method [Topics in Catalysis 53 (2010) 700-706] Sunho Jung, Ai Suzuki, Hideyuki Tsuboi, Nozomu Hatakeyama, Akira Endou, Hiromitsu Takaba, Momoji Kubo, and Akira Miyamoto
475. Adsorption and Dissociation of Molecular Hydrogen on Pt/ CeO_2 Catalyst in the Hydrogen Spillover Process: A Quantum Chemical Molecular Dynamics Study [Applied Surface Science 256 (2010) 7643-7652] Farouq Ahmed, Md. Khorshed Alam, Ryuji Muira, Ai Suzuki, Hideyuki Tsuboi, Nozomu Hatakeyama, Akira Endou, Hiromitsu Takaba, Momoji Kubo and Akira Miyamoto

476. Study of Reduction Processes over Cerium Oxide Surfaces with Atomic Hydrogen using Ultra Accelerated Quantum Chemical Molecular Dynamics [Applied Surface Science 257 (2010) 1383-1389] Md. Khorshed Alam, Farouq Ahmed, Ai Suzuki, Hideyuki Tsuboi, Nozomu Hatakeyama, Akira Endou, Hiromitsu Takaba, Momoji Kubo, Akira Miyamoto
477. A Computational Chemistry Study on Friction of h-MoS₂. Part II. Friction Anisotropy, [Journal of Physical Chemistry B 114 (2010) 15832-15838] Tasuku Onodera, Yusuke Morita, Ryo Nagumo, Ryuji Miura, Ai Suzuki, Hideyuki Tsuboi, Nozomu Hatakeyama, Akira Endou, Hiromitsu Takaba, Fabrice Dassenoy, Clotilde Minfray, Lucile Joly-Pottuz, Momoji Kubo, Jean-Michel Martin, Akira Miyamoto
478. Restoration of p53–DNA Interaction Loss upon R273H Mutation by CP-31398: An Ultra Accelerated Quantum Chemical Molecular Dynamics Approach, [Medicinal Chemistry Research (2010) 1-6] Shah Md. Abdur Rauf, Kamlesh Kumar Sahu, Hideyuki Tsuboi, Nozomu Hatakeyama, Akira Endou, Hiromitsu Takaba, Carlos A. Del Carpio, Akira Miyamoto
479. Multi-Scale Theoretical Study of Sintering Dynamics of Pt for Automotive Catalyst. [SAE International Journal of Fuels and Lubricants 2 (2010) 337-345] Ai Suzuki, Ryo Sato, Katsuyoshi Nakamura, Kotaro Okushi, Hideyuki Tsuboi, Nozomu Hatakeyama, Akira Endou, Hiromitsu Takaba, Momoji Kubo, Mark C. Williams, Akira Miyamoto
- [2011]
480. Computational Study on Carrier Injection in Ca/Poly (9,9'-dioctylfluorene) Interface by Using Quantum Chemistry and Monte Carlo Methods [Japanese Journal of Applied Physics, 50 (2011) 04DK02] Itaru Yamashita, Hiroaki Onuma, Ryo Nagumo, Ryuji Miura, Ai Suzuki, Hideyuki Tsuboi, Nozomu Hatakeyama, Akira Endou, Hiromitsu Takaba, Momoji Kubo, and Akira Miyamoto
481. Multiscale Simulation of Dye-Sensitized Solar Cells Considering Schottky Barrier Effect at Photoelectrode [Japanese Journal of Applied Physics, 50 (2011) 04DP06] Mari Onodera, Ryo Nagumo, Ryuji Miura, Ai Suzuki, Hideyuki Tsuboi, Nozomu Hatakeyama, Akira Endou, Hiromitsu Takaba, Momoji Kubo, and Akira Miyamoto

482. Theoretical Study on Effect of SiC Crystal Structure on Carrier Transfer in Quantum Dot Solar Cells. [Japanese Journal of Applied Physics, 50 (2011) 04DP05] Sho Hirose, Itaru Yamashita, Ryo Nagumo, Ryuji Miura, Ai Suzuki, Hideyuki Tsuboi, Nozomu Hatakeyama, Akira Endou, Hiromitsu Takaba, Momoji Kubo, and Akira Miyamoto
483. Influence of surface chemistry on the electronic properties of graphene nanoflakes [Chemical Physics Letters, v. 503, iss. 1-3, p. 91-96. (2011)] Chutia, Arunabhiram; Cimpoesu, Fanica; Tsuboi, Hideyuki; Miyamoto, Akira
484. Ionomer content in the catalyst layer of polymer electrolyte membrane fuel cell (PEMFC) : Effects on diffusion and performance [International Journal of Hydrogen Energy] Ai Suzuki, Unal Sen, Tatsuya Hattori, Ryuji Miura, Ryo Nagumo, Hideyuki Tsuboi, Nozomu Hatakeyama, Akira Endou, Hiromitsu Takaba, Mark C. Williams, Akira Miyamoto
485. Modeling of Hydrogen Vacancy for Dissociative Adsorption of H₂ on Pd (111) Surface by A Quantum Chemical Molecular Dynamics [Catalysis Today 164 (2011) 16-22] Farouq Ahmed, Md. Khorshed Alam, Ryuji Miura, Ai Suzuki, Hideyuki Tsuboi, Nozomu Hatakeyama, Akira Endou, Hiromitsu Takaba, Momoji Kubo, and Akira Miyamoto
486. Surface Reduction Processes of Cerium Oxide Surfaces by H₂ Using Ultra Accelerated Quantum Chemical Molecular Dynamic Study [Catalysis Today 164 (2011) 9-15] Md. Khorshed Alam, Farouq Ahmed, Ryuji Miura, Ai Suzuki, Hideyuki Tsuboi, Nozomu Hatakeyama, Akira Endou, Hiromitsu Takaba, Momoji Kubo, Akira Miyamoto
487. Exergetic Efficiency Rate of Change and Fuel Cell Degradation [ECS Transactions Vol30 (2011) 207-215] M. Williams, A. Suzuki, and A. Miyamoto

Ⅲ. 口頭発表（学会報告など）

国際会議招待講演等

[1992]

1. Role of Zeolite Framework in CuZSM-5 Catalysts for Direct Decomposition of NO_x as Investigated by Molecular Dynamics and Computer Graphics
[203rd American Chemical Society Meeting Catalysis Session]
(San Francisco, USA, April 2-5, 1992)
Invited Paper
 2. Structure and Dynamics of Heterogeneous Catalysts as Investigated by Molecular Dynamics and Computer Graphics
[The Second International Conference & Exhibition on Computer Applications to Materials and Molecular Science and Engineering]
(Yokohama, Japan, September 22-25, 1992)
Invited Paper
 3. Structure and Dynamics of Heterojunction in Epitaxial Films as Investigated by Molecular Dynamics and Computer Graphics
[The 6th International Conference on Ferrites Satellite Conference in Kyoto]
(Kyoto, Japan, October 4-7, 1992)
Invited Paper
 4. Application of Computer Graphics and Molecular Dynamics to Catalyst Design
[The 7th Seminar on Science and Technology ROC-Japan Joint Workshop on Catalysis]
(Taipei, ROC, December 10-11, 1992)
Invited Paper
- [1993]
5. [The 7th International Seminar on Frontier Technology Computational Chemistry and Its Macro-Micro Bridge]
(Kanagawa, Japan, May 26-28, 1993)
Invited Paper
 6. Structure and Dynamics of Ion-exchanged Zeolites as Investigated by Molecular Dynamics and Computer Graphics
[International Symposium on Zeolites and Microporous Crystals]
(Nagoya, Japan, August 22-25, 1993).
Invited Paper
 7. Application of Molecular Dynamics and Computer Graphics to Catalyst Design
[12th International Conference on Catalysis - The Taniguchi Foundation -]
(Osaka, Japan, October 31-November 5, 1993).
Invited Paper

8. Structure and Dynamics of Exchanged Cations in Zeolites as Investigated by Molecular Dynamics and Computer Graphics

[International Symposium of Acid-Base Catalysis II]

(Sapporo, Japan, December 2-4, 1993)

Invited Paper

[1995]

9. Theoretical Models in Catalyst Design

[Discussion Forum of Polish Academy of Science]

(Mogilany, Poland, October, 11-13, 1995)

Invited Paper

[1996]

10. Development and Application of Integrated Computational Chemistry System for the Design of Heterogeneous Catalysts and Nanostructured Materials

[India-Japan Joint Seminar on Computational Materials Science]

(Hyderabad, India, October, 21-22, 1996)

Invited Paper

[1997]

11. Integrated Computational Chemistry System for the Design of Heterogeneous Catalysts and Microporous Materials

[17th Tsukuba Symposium - Challenge towards Large-Scale Computer Simulations: Complex Processes and Novel Materials]

(Tsukuba, Japan, February, 20, 1997)

Invited Paper

12. Application of Integrated Computational Chemistry System to the Design of Inorganic Membranes

[213th American Chemical Society Meeting]

(San Francisco, USA, April, 13-17, 1997)

Invited Paper

13. Integrated Computational Chemistry System for the Design of Inorganic Membranes

[The 1997 Fifteenth Annual Membrane Technology/Separations Planning Conference]

(Newton, USA, October 27-29, 1997)

[1998]

14. Integrated Computational Chemistry Study for Zeolite Microporous Materials
[International Catalysis Symposium on "Frontier and Tasks of Catalysis Towards Next Century"]
(Kyoto, Japan, March 20-21, 1998)
Invited Paper
15. Methane Activation on the Heterogeneous Active Sites
[215th American Chemical Society Meeting]
(Dallas, USA, March 29 - April 2, 1998)
Invited Paper
16. Periodic First-Principles Study on Active Site of V_2O_5 Surface and Mechanism of Selective Catalytic Reduction of NO by NH_3
[Impact of Computer to Catalyst Research and Development 2]
(Kyoto, Japan, July 26-28, 1998)
Invited Paper

[1999]

17. Combinatorial Computational Chemistry Approaches to the Design of Heterogeneous Catalysts
[National Chemical Laboratory Golden Jubilee Conference]
(Pune, India, January 18-20, 1999)
Invited Paper
18. Simulation Study of Permeation through the Microporous Membrane
[Italy-Japan Workshop on Catalytic Membrane Reactors and Integrated Membrane Operations]
(Centaro, Italy September 23-27, 1999)
Invited Paper

[2000]

19. Combinatorial Computational Chemistry Approach to the Design of Catalysts
[SPIE's International Symposium on Integrated Optoelectronic Devices (Optoelectronics 2000)]
(San Jose, USA, January 22-28, 2000)
Invited Paper

20. Most Recent Progress in Integrated Computational System for Catalysts and Materials Design
[ICS-UNIDO-NCL Workshop on Clean Catalytic Processes for Fine Chemicals and Pharmaceuticals]
(Pune, India, February 7-9, 2000).
Invited Paper
21. Combinatorial Computational Chemistry Methods for Catalysts and Materials Design
[Tenth Conference on Combinatorial Chemistry, Japan]
(Osaka, Japan April 24-25, 2000)
Invited Paper
22. Integrated Computational Chemistry Methods for Catalyst Design
[International Symposium Catalysis in XXI Century: from Quantum Chemistry to Industry]
(Krakow, Poland, May 4-7, 2000)
Invited Paper
23. Theoretical Design of Heterogeneous Catalysts: Combinatorial Computational Chemistry Approach
[The First Japan-US Workshop on Combinatorial Material Science and Technology]
(Maui, USA, October 1-3, 2000)
Invited Paper
24. Atomistic and Electronic Nature of Molecular Tribology on Solid Surfaces as Investigated by Integrated Computational Chemistry System
[Tribochemistry Tsukuba 2000]
(Tsukuba, Japan, October 27, 2000)
Invited Paper
25. Periodic First-Principle Density Functional Approach to the Design of Catalysts
[Pacifichem 2000]
(Honolulu, USA, December 14-19, 2000)
Invited Paper

26. Dynamics of Adsorbed Molecules on a Pd Surface Investigated by Ab-Initio Hybrid Molecular Dynamics Method
[International Conference on Elementary Processes in Molecule-Metal Surface Interaction]
(San Juan, Puerto Rico, November 11-15, 2000)
Invited Paper

[2001]

27. Combinatorial Computational Chemistry Approaches to Catalyst Screenings: A New Concept for the 21st Century
[Fifteenth Indian National Symposium on Catalysis and Second Conference of the Indo-Pacific Catalytic Association]
(Pune, India, January 23 - 25, 2001)
Plenary Lecture
28. Future of Computer-Aided Materials Design
[Ninth International Conference on Properties and Phase Equilibria for Product and Process Design]
(Kurashiki, Japan, May 20 - May 25, 2001)
Invited Paper
29. Development of New Program for Combinatorial Computational Chemistry: Its Application to Methane Activation
[12nd CRC International Symposium on "Advanced Chemical Conversion of Methane"]
(Sapporo, Japan, November 18-20, 2001)
Invited Paper
30. Proposal of New Concept "Combinatorial Computational Chemistry" and Its Application to Catalyst Design
[2001 Materials Research Society Fall Meeting]
(Boston, USA, November 26-30, 2001)
Invited Paper

[2002]

31. Development and Applications of Accelerated Quantum Chemical Molecular Dynamics Method for Degradation Dynamics of Organic Lubricants under High Temperatures and Pressures
[2nd International Workshop on Microtribology]
(Ishigaki, Japan, April 16-19, 2002)
Invited Paper

32. Development of Novel Methodology for Combinatorial Computational Chemistry
[14th Conference on Combinatorial Chemistry, Japan]
(Osaka, Japan, April 22-23, 2002)
Invited Paper
 33. Design of Novel Functions of Ultrafine Particles by Computational Chemistry Methods
[2002 IFPRI Annual General Meeting]
(Sendai, Japan, July 14-18, 2002)
Invited Paper
 34. Computational Methods for the Design of Zeolitic Materials
[2nd FEZA Conference]
(Taormina, Italy, September 1-5, 2002)
Plenary Lecture
- [2003]
35. Development of Integrated Computational Chemistry System for the Design of Zeolite Materials
[International Symposium on Zeolites and Microporous Crystals (ZMPC2003)]
(Sapporo, Japan, August 3-6, 2003)
Invited Paper
 36. Application of Computational Chemistry Methods for Industry Innovation
[The 8th IUMRS International Conference on Advanced Materials]
(Yokohama, Japan, October 8-13, 2003)
Invited Paper
 37. Development of Integrated Combinatorial Computational Chemistry and Its Application to Material Design
[The 8th IUMRS International Conference on Advanced Materials]
(Yokohama, Japan, October 8-13, 2003)
Invited Paper
 38. Application of Integrated Computational Chemistry Approach to the Design and Development of Catalysts and Materials - The State of the Art
[India-Japan Seminar on New Materials]
(Yokohama, Japan, October 12, 2003)
Invited Paper

[2004]

39. Computational Methods for Nanotribology and Tribochemical Reactions
[3rd International Conference on "Computational Modeling and Simulation of Materials"]
(Sicily, Italy, May 29-June 4, 2004)
Invited Paper

[2005]

40. Combinatorial Computational Chemistry for Industrial Innovations
[The 4th Asia-Pacific Chemical Reaction Engineering Symposium]
(Gyeongju, Korea, June 12-15, 2005)
Plenary Lecture
41. Integrated Computational Chemistry System for the Material Design of Plasma Display
[The 12th International Display Workshops in conjunction with Asia Display 2005]
(Takamatsu, Japan, December 6-9, 2005)
Invited Paper

[2006]

42. Computational Chemistry Methods for the Design of Microporous Materials for Industrial Applications
[International Symposium on Zeolites and Microporous Crystals 2006]
(Yonago, Japan, July 30-Aug 2, 2006)
Keynote Lecture
43. Theoretical Study of PDP Materials
[Pre-Workshop of the 6th International Meeting on Information Display and the 5th International Display Manufacturing Conference (IMID/IDMC 2006)]
(Daegu, Korea, August 22, 2006)
Keynote Lecture
44. Theoretical Study of PDP Materials
[The 6th International Meeting on Information Display and the 5th International Display Manufacturing Conference (IMID/IDMC 2006)]
(Daegu, Korea, August 22-25, 2006)
Invited Lecture

[2007]

45. Multi-Level Combinatorial Computational Chemistry for Industrial Innovation
[The 4th Asian Consortium on Computational Materials Science]
(Seoul, Korea, September 13-16, 2007)
Invited Lecture
46. Multi-Level Combinatorial Computational Chemistry for Nano-Scale Flow
Dynamics in Highly Coupled Systems
[The Fourth International Conference on Flow Dynamics]
(Sendai, Japan, September 26-28, 2007)
Keynote Lecture

[2008]

47. Multi-Level Combinatorial Computational Chemistry for Future Electron Devices
[International Meeting for Future of Electron Devices, Kansai (IMFEDK2008)]
(Osaka, Japan, May 22-23, 2008)
Invited Lecture
48. Experiments Integrated Multilevel Computational Chemistry Methods for the
Application to PDP Protecting Layer
[IMID/IDMC/Asia Display 2008]
(Ilsan, Korea, October 13-17, 2008)
Invited Lecture
49. Multi-level Combinatorial Computational Methods for Industrial Innovations
[1st NanoThailand Symposium]
(Bangkok, Thailand, November 6-8, 2008)
Invited Lecture
50. Theoretical approach to amine reaction with integrated computational chemistry
methods
[CSIRO-RITE 科学技術シンポジウム]
(Kyoto, Japan, May 26, 2009)
Invited Lecture
51. Experiment Integrated Multi-Level Computational Chemistry for Tribology
[Tribochemistry Kyoto 2009]
(Kyoto, Japan, Sept. 2-4, 2009)
Invited Lecture

52. New Horizons in Tribology: The Computational Chemistry Paradigm
[World Tribology Congress 2009]
(Kyoto, Japan, Sept. 6-11, 2009)
53. Multilevel Combinatorial Computational Chemistry Approach for Dielectric Materials
[14th US-Japan Seminar]
(Oregon, USA, October 11-14, 2009)
Plenary Lecture
54. Computational Chemistry as Practical Solution to Industrial Problems: Present States and Future Prospects
[The 13th International Conference on Theoretical Aspects of Catalysis]
(Miyagi, Japan June 21, 2010)
Plenary Lecture
55. Enabling and investigative tools: theory, modeling, and simulation Moderators
[Long-term Impacts and Future Opportunities for Nanotechnology" US-Japan-Korea-Taiwan Workshop]
(Ibaraki, Japan , July 26, 2010)
Invited Lecture

国内会議招待講演等

※1994年以前の講演は省略

[1995]

1. 「コンピュータ支援触媒設計の現状と展望」
化学工学会 CE クラブ講演会
1995年 5月24日, 東京
2. 「コンピュータ支援材料設計」
結晶成長研究会
1995年 6月 5日, つくば
3. 「コンピュータ化学からみたマイクロポーラス系の特徴」
物性研研究会
1995年 6月28日～6月29日, 東京
4. 「コンピュータ化学からみた触媒の理想」
物質研シンポジウム
1995年 7月13日～14日, つくば

5. 「表面および触媒研究への分子動力学法の応用」
計算化学サマーセミナー
1995年7月19日～7月21日, 富士
6. 「金属表面の微細構造と成長機構の分子シミュレーション」
酸化物エレクトロニクス研究会
1995年9月12日, 東京
7. 「セラミックスの計算化学」
セラミックス大学
1995年10月7日, 東京
8. 「CO₂のゼオライト上への吸着と膜分離の分子シミュレーション」
CO₂固定化研究セミナー
1995年11月28日, 東京
9. 「コンピュータによる触媒分子論」
化学工学の進歩講習会
1995年11月28日～11月30日, 名古屋
10. 「触媒設計の夢と課題」
夢に挑戦する計算機材料設計シンポジウム
1995年11月29日, 東京
11. 「コンピュータ支接触媒設計の現状と展望」
触媒学会北海道地区講演会
1995年12月12日, 函館

[1996]

12. 「触媒設計のためのコンピュータケミストリー」
第6回反応化学シンポジウム
1996年1月12日, 仙台
13. 「分子動力学法とトライボケミストリー」
第14回トライボケミストリー研究会
1996年3月27日, 東京
14. 「バーチャルリアリティ技術統合触媒設計支援システム」
第2回物質・材料設計のための仮想実験技術シンポジウム
1996年5月17日, 東京, 大手町フィナンシャルセンター

15. 「コンピューター支援触媒設計」
第12回田丸コンファレンス触媒化学の新展開
1996年5月31日, 伊豆, 熱川ハイッ
16. 「CCSの現状と将来」
学振プロセスシステム工学研究会
1996年7月18日, 東京, 弘済会館
17. 「バーチャルリアリティー統合コンピュータ化学システムの開発と触媒・材料設計への応用」
近畿化学協会コンピュータ化学部会
1996年9月13日, 大阪, 化学技術センター
18. 「コンピュータケミストリを如何に触媒設計に役立てるか」
触媒討論会研究発表会
1996年10月11日, 福岡, 九州大学箱崎キャンパス
19. 「量子化学, 分子動力学, コンピュータ・グラフィックスによる統合的アプローチ」
文部省重点領域研究「特殊反応場の触媒化学」第5回サテライトセミナー
1996年11月1日, 倉敷 加計国際学術交流センター
20. 「超精密構造解析とコンピュータ化学」
北大触媒化学研究センター第8回研究発表会
1996年11月15日, 札幌, 北海道大学触媒化学研究センター

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21. 「コンピュータケミストリーによるゼオライト研究の現状と展望」
平成9年度ゼオライト研究会総会
1997年1月24日, 蔵前工業会館
22. 「コンピュータケミストリーは化学産業にどう貢献できるか」
第21回革新領域セミナー
1997年1月29日~31日, 生産性国際交流センター(湘南国際村)
23. 「統合コンピュータ化学システムの構築とファインセラミックスへの応用」
ファインセラミックス研究会
1997年10月23日, 東北工業技術研究所
24. 「分子シミュレーションの膜技術への応用」
最近の化学工学-膜技術の動向と将来展望-
1997年11月7日, 早稲田大学国際会議場第3会議室

25. 「コンピュータ化学による環境保全・汚染物質の分子構造」
粉体工学シンポジウム
1997年11月27日, 東北大学 (片平)

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26. 「ケイ酸塩鉱物へのコンピューターケミストリーの応用」
スメクタイト研究会第15回講演会
1998年5月22日, 仙台サンプラザホテル
27. 「固体触媒シミュレーション技術の現状とメタン活性化への応用」
資源環境技術研究所第14回研究講演会
1998年7月3日, 東京石垣記念ホール
28. 「Integrated Computational Chemistry System for the Crystal Growth and Chemical Reactions on Solid Surfaces」
1998年8月5日～6日, 第9回CRESTダイヤモンド表面研究会
29. 「触媒表面反応ダイナミックスの計算化学」
触媒討論会
1998年9月16日～19日, 愛媛大学
30. 「コンピュータ化学による固体表面研究の現状と展望」
日本化学会コロイド界面化学討論会
1998年9月24日～26日, 千葉大学
31. 「計算科学によるマテリアルライブラリー設計」
無機材料のコンビナトリアルケミストリー研究会
1998年9月29日, 東京工業大学長津田キャンパス
32. 「トライボロジーへの統合計算化学手法の応用」
日本機械学会 IIP 部門講習会
1998年11月5日, 東京工業大学百年記念会館
33. 「コンピュータ支援触媒・材料設計」
ニューフロンティア材料研究会
1998年11月21日, 大阪府立大学
34. 「固体表面反応ダイナミックスの計算化学」
第18回表面科学講演大会
1998年12月1日～3日, 早稲田大学

35. 「コンビナトリアル計算化学と触媒研究への応用」
東北地区触媒講演会
1998年12月21日, 東北大学

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36. 「固体表面の微細構造と化学反応ダイナミクス：計算化学からのアプローチ」
第22回表面科学研究会
1999年2月3日～4日, つくば, 金属材料技術研究所
37. 「計算科学を用いた触媒研究」
精密工学会超精密加工専門委員会第38回研究会
1999年4月21日, 大阪ガーデンパレス
38. 「触媒・無機機能材料分野で計算科学活用法：成功のためのノウハウ」
高分子計算機科学研究会
1999年7月8日, 東京大学
39. 「触媒・材料設計のためのコンビナトリアル計算化学：密度汎関数法の役割」
計算化学サマーセミナー
1999年7月21日～23日, 箱根
40. 「コンビナトリアル計算科学による材料開発」
第60回応用物理学会学術講演会
1999年9月1日～4日, 神戸, 甲南大学
41. 「摩擦の分子動力学によるシミュレーション」
第52回コロイドおよび界面化学討論会
1999年10月16日～18日, 盛岡
42. 「コンピュータと化学」
すいよう会
1999年11月4日, 東京
43. 「フロン, ダイオキシン研究が求めるコンピュータ化学の方向」
第9回ハロゲン関連物質触媒研究発表会
1999年12月10日, 大分, 大分大学工学部
44. 「統合コンピュータ化学システムによる材料科学研究」
東京工業大学応用セラミックス研究所講演会
1999年12月13日, 神奈川, 東京工業大学応用セラミックス研究所

45. 「統合コンピュータ化学システムによるリチウム二次電池正極材料の分子設計」
新炭素系電子材料研究会
1999年12月14日, 京都, 基礎化学研究所

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46. 「高性能二次電池の分子設計：コンピュータケミストリーからのアプローチ」
電気化学会東北支部第31回セミコンファレンス
2000年1月13日～14日, 盛岡, ホテル紫苑
47. 「統合化コンピュータ化学システム」
日本学術振興会ナノプローブテクノロジー第167委員会
2000年1月25日, 東京
48. 「計算化学が切り開く新しい化学工学」
化学工学会専7-5技術開発法&工業化法専門委員会第6回定例委員会
2000年1月28日, 東京
49. 「高速化量子分子動力学プログラムによる表面反応ダイナミックス」
第28回表面科学研究会
2000年2月2日～3日, つくば, 金属材料技術研究所
50. 「統合コンピュータ化学システムによる化学電池材料の分子設計」
第4回化学電池材料研究会
2000年2月24日, 東工大
51. 「統合コンピュータ化学システムによる環境技術のための吸着・表面反応の研究」
弥生研究会
2000年3月3日, 東大工, 東京
52. 「ナノスペース内分子挙動のコンピュータシミュレーション」
第4回機能構造と分析化学シンポジウム
2000年6月30日, 東北大, 仙台
53. 「マイクロ・メソ多孔体における計算化学の新展開」
第86回触媒討論会
2000年9月19日～22日, 鳥取大, 鳥取

54. 「分子シミュレーションの基礎と応用」
コンピュータシミュレーション活用術講習会
2000年11月30日, 東北大学, 仙台
55. 「コンピュータ化学を通して見た触媒の未来像」
東北地区触媒講演会
2000年12月1日, 東北大学, 仙台

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56. 「コンビナトリアル計算化学による触媒設計」
日本化学会第79春季年会
2001年3月28日～31日, 甲南大学, 神戸
57. 「分子シミュレーション手法によるせん断場での有機分子の潤滑挙動解析」
ファイル記憶のトライボロジー研究会
2001年9月14日, 三菱化学, 東京
58. 「化学ソフトウェア大国への戦略と展望」
化学ソフトウェア学会年会「2001研究討論会」
2001年9月29日～30日, 埼玉大学, 浦和

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59. 「コンピュータが明かす魅惑的な触媒の世界」
日本化学会第81春季年会
2002年3月26日～29日, 早稲田大学, 東京
60. 「ナノスペースの分子挙動のシミュレーション」
特定領域研究B「液液界面ナノ領域の化学」公開シンポジウム
2002年7月29日～30日, 東北大学, 仙台
61. 「固体表面上での励起反応ダイナミックスのための高速化量子分子動力学法の開発と応用」
東北物理化学コロキウム「物理化学・理論化学と分光学のニューフロンティア」
2002年11月1日～2日, 東北大学, 仙台
62. 「コンビナトリアル計算化学のための新手法の開発」
第1回東北大学化学系21世紀COEシンポジウム
2002年11月7日, 勝山館, 仙台

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63. 「コンピ計算化学のための新手法の開発と応用」
応用物理学会，神奈川県，神奈川県
2003年3月27日～30日
64. 「コンビナトリアル計算化学のための新手法の開発」
新化学発展協会先端化学技術部会講演会，新化学発展協会，東京
2003年6月18日
65. 「分子動力学法による潤滑材の挙動解析」
日本塑性加工学会塑性力学分科会
2003年6月27日
66. 「分子動力学による摩擦摩耗現象の解明の試み」
トライボロジーフォーラム2003
2003年7月17日～18日，厚生年金ハートピア熱海，熱海
67. 「コンピュータ支援触媒設計の現状と展望」
触媒学会箱根セミナー
2003年7月30日～8月1日
68. 「量子分子動力学の現状と将来」
21世紀 COE ナノテクノロジー基盤機械科学フロンティア第1回拠点内シンポジウム
2003年10月17日，東北大学，仙台
69. 「コンビナトリアル計算化学と燃料電池技術：現状と展望」
第3回生活環境系特別研究体フォーラム「燃料電池のナノテク・ナノサイエンス」
2003年10月24日，産総研関西センター，大阪
70. 「企業における技術革新を実現する計算化学」
「高密度 DVD 用集光機能ナノガラス薄膜の開発」学術講演会
2003年10月27日，(株)日立製作所日立研究所，日立

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71. 「無機複雑分子系の計算化学」
第21回無機・分析化学コロキウム
2004年6月18日～19日，蔵王ハイツ，蔵王

72. 「コンビナトリアル計算化学の最近のトピックスについて」
第17期 CAMM フォーラム本例会
2004年8月6日, 虎ノ門パストラル, 東京

73. 「ナノガラスシミュレーション」
シミュレーション技術学術講演会
2004年8月11日, 日立製作所日立研究所, 日立

74. 「コンビナトリアル計算化学」
コンビナトリアルテクノロジーフォーラム
2004年8月26日, 東京大学山上会館, 東京

75. 「産業革新のためのコンピュータ化学現状と展望」
CAC フォーラム, 秋保グランドホテル, 仙台
2004年10月4日, 5日

76. 「実用材料設計のためのコンビナトリアル計算化学」
第1回 PDP フォーラム: 駒場 PDP 工学領域研究会
2004年11月26日, 東京大学生産技術研究所, 東京

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77. 「コンビナトリアル計算化学: 新手法の開発とその産業応用」
近畿化学協会「コンピュータ化学部会」例会
2005年2月22日, 大阪科学技術センター, 大阪

78. 「統合化計算化学システムによる PDP 保護膜材料の理論的設計」
日本化学会第85春季年会
2005年3月26日~29日, 神奈川大学横浜キャンパス, 横浜

79. 「統合化コンピュータ化学システムによる薬学研究へのアプローチ」
日本薬学会第125年会
2005年3月29日~31日, 東京臨海副都心, 東京

80. 「PDP 材料シミュレーション」
次世代ディスプレイ寄附研究部門2周年記念シンポジウム
2005年11月25日, 東京大学生産技術研究所, 東京

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81. 「セラミックスの機能予測シミュレーションの最前線」
「ナノテクノロジー材料技術~実用化への期待~」講演会
2006年1月23日, ファインセラミックスセンター, 名古屋

82. 「産業革新のためのコンピュータ化学：現状と将来展望」
日本機械学会東北支部第41期総会・講演会
2006年3月14日, 青葉記念会館, 仙台
83. 「産業革新のための実践的マルチレベル・コンビ計算化学：方法論と具体例」
第20回分子シミュレーション討論会
2006年11月27日～29日, 仙台国際センター, 仙台
84. 「統合化計算化学手法における燃料電池開発」
水素・燃料電池ワークショップ in KYOTO 2006
2006年12月6日, 京都

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85. 「計算科学によるトライボロジー現象の解明」
トライボロジー先端講座
2007年2月16日, 東京理科大学森戸記念館, 東京
86. 「産学連携のための実践的コンピュータ科学：具体的方法と成功事例」
産学官ニーズ対応連環型交流会
2007年2月20日, ウェルシティ長崎, 長崎
87. 「トライボロジー研究が育む実践的コンピュータ化学の未来像」
トライボケミストリー討論会
2007年3月16日, 仙台
88. 「統合化計算化学システムによる PDP 材料の理論設計」
日本化学会第87春季年会
2007年3月25日～28日, 関西大学千里山キャンパス, 大阪
89. 「産業革新のための実践的コンピュータ化学：方法論と成功例」
日本化学会第1回関東支部大会
2007年9月27日～28日, 首都大学東京八王子キャンパス, 東京
90. 「理論化学によるナノスケルトンの設計と応用利用」
第60回コロイドおよび界面化学討論会
2007年9月20日～22日, 信州大学理学部, 松本
91. 「マルチスケール／マルチフィジックスシミュレーションのための新計算化学手法の開発と実践的産業課題への応用」
NEC ユーザフォーラム SP 研ワークショップ
2007年12月5日, 東京ビッグサイト, 東京

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92. 「産業革新のための実践的コンピュータ化学：触媒研究への応用」
第101回触媒討論会
2008年3月28日～29日, 船堀タワーホール, 東京
93. 「産業革新のための実践的コンピュータ化学：現状と展望」
化学工学会第40回秋季大会
2008年9月24日～26日
94. 「シミュレーションの専門的見地からあるべきナノ計測との連動方法。産学
の間の「死の海」を乗り切るために必要な方向性。」
JST 深掘ワークショップ 見えないものを見る - Observation と Modeling と
の協奏 -
2009年1月8日
95. 「産業革新のための実践的コンピュータ化学：現状と将来展望」
日本コンピュータ化学会2009春季年会 学会賞受賞講演
2009年5月21日
96. 活性点の解析に役立つキャラクタリゼーション
触媒学会セミナー
2010年10月15日
97. 固体内励起エネルギー移動に関する電子状態計算
応用物理学会励起ナノプロセス研究会
2010年11月2日
98. Multi-level Computational Chemistry Methods for Green and Sustainable
Chemistry
鳥取大学講演会
2010年11月13日
99. 理論的計算化学から見た電池の可能性
科学技術未来戦略ワークショップ「次々世代二次電池・蓄電デバイス技術」
2011年1月27日
100. レアアース～NEDO 自動車触媒セリウム削減・代替研究開発
東北の自動車産業・次世代移動体システムの未来像を描くための産学官連携
促進セミナー
2011年5月25日

101. コンピュータが創る新しい化学
夢ナビライブ2011 (大阪会場)
2011年7月12日

102. コンピュータが創る新しい化学
夢ナビライブ2011 (東京会場)
2011年7月16日