OAK RIDGE NATIONAL LABORATORY

OPERATED BY MARTIN MARIETTA ENERGY SYSTEMS, INC.
POST OFFICE BOX 2008, OAK RIDGE, TENNESSEE 37831-6285

ORNL

FOREIGN TRIP REPORT

FTR-3755

DATE: September 24, 1990

SUBJECT: Report of Foreign Travel of S. H. Liu, Corporate Fellow,
Solid State Theory Section, Solid State Division, ORNL

TO: Alvin W. Trivelpiece

ORNL/FTR--3755

FROM: S. H. Liu

DE91 000383

PURPOSE: To attend a "Working Party on Electrochemistry: Condensed Matter, Atomic and Molecular Aspects" and to present an invited lecture entitled "Fractal Electrodes: Interplay of Physics and Geometry-I."

SITES VISITED: 9/3-8/90 Trieste, Italy Working Party on
Electrochemistry

ABSTRACT: The author was one of 26 invited lecturers to discuss the latest developments of the physical aspects of electrochemistry. He interacted extensively with other lecturers and many participants from developing countries. He also visited with the Director of the Italian Synchrotron Radiation Source now under construction in Trieste, Italy.

DISCLAIMER

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

The Working Party on Electrochemistry was organized by the International Centre for Theoretical Physics under the Directorship of A. A. Kornyshev, Academy of Sciences of the USSR, A. N. Frumkin Institute of Electrochemistry, Moscow, USSR. The purpose of the Working Party was to bring together first-world and third-world scientists to discuss the latest ideas and results in the physics and chemistry of the electrode and electrolyte system. The lecturers were selected for their timely contributions to this field, and the participants were mostly physicists and physical chemists from developing countries. The International Centre for Theoretical Physics, Trieste, Italy, provided financial support for the project except travel expenses, which were borne by the individual members' home institutions. The Working Party lasted for two weeks, and the author was present during the second week. There were 26 lecturers and 35 participants present at various times.

The main topics under discussion at the Working Party were: (1) theory of liquids and solutions; (2) the electrochemical interface (structure and electric properties, electrodynamics); (3) elementary act of charge transfer reactions and electrochemical kinetics; and (4) fundamental ideas in applied electrochemistry. There were approximately 40 scheduled lectures evenly distributed among the 4 topics. Impromptu, short seminars were inserted into the schedule wherever feasible to give third-world scientists the chance to present their works. Unfortunately, none made use of this opportunity, and the seminars were all given by scientists from developed countries.

The author's contributions to this field are covered in the second topic—the structure and electric properties of the interface. He was gratified to hear that his early contribution, the relevance of surface electronic states on the metal electrode to the physical and chemical properties of the interface, was mentioned repeatedly by other lecturers. The ideas and results published by the author and his coworkers in four laboratories in the U. S. and Europe have become standard literature and are explored by many scientists as tools for their investigations of surface adsorption of chemical species. His more recent contribution concerns the fractal nature of the interface and its influence on the interfacial impedance. This problem is of basic interest to industrial scientists who engage in the design and manufacture of batteries and other electrolytic devices. He was asked to lecture on this problem, and two other

lecturers discussed other implications of fractal geometry. He also presented his latest work, carried out at ORNL in collaboration with T. Kaplan, Solid State Division, and L. J. Gray, Engineering Physics and Mathematics Division, on the self-generated fractal distribution of vacancies in solid electrolytes during the conduction process. This new concept may explain the unusual frequency dependence of the electrical impedance of fast-ion conductors. Consequently, it may also have practical implications in electrolytic devices which utilize solid electrolytes. The theoretical program at ORNL to study the relation of fractal geometry and electrochemistry was stimulated by the experimental finding of J. B. Bates, Solid State Division.

The author could see incremental to significant progress in the last two years in all topics under discussion. The computer simulation method is playing an increasing role in the understanding of liquid structure and chemical kinetics and may become the method of choice in the future because analytical theories have been found to be intractable. The enhanced Raman effect, discovered nearly 20 years ago, continues to be the most popular tool for microscopic investigations of surface absorption, although newly developed optical methods, such as surface state absorption and second-harmonic generation, have become mature and competitive. Semiconductors are preferred over metal by many as the electrode materials in many energy conversion devices. On the other hand, the theory of the semiconducting electrode is very poorly developed. The author left the meeting with a tinge of regret that he does not have more time and energy to tackle these challenging problems.

The relaxed atmosphere of the Centre, in general, and the Working Party, in particular, encouraged active interactions between members of the Party. There were extensive discussions among the lecturers, and all felt that the meeting was productive and highly worthwhile. On the other hand, a few scientists from developed countries, including the Director of the Working Party, shared the author's uneasy feeling that the meeting failed to achieve its primary purpose, namely to bridge the considerable gap between first-world and third-world scientists. Although 35 participants registered for the meeting, seldom more than 20 were present at any given lecture. In contrast, all lecturers present attended each others' lectures. There were lively discussions

after every lecture, but these involved only the lecturers. During breaks and after dinner one would find small groups engaged in further discussions of the day's lectures. But the groups were completely segregated, and the author witnessed little interaction between scientists from developed and developing countries. What the Working Party has accomplished is to expose the scientists from developing countries to the way science is done in developed countries. The author interacted with many scientists from Asian countries, and they were concerned about such questions as how science is funded, how an individual scientist's performance is judged, how to smooth over rivalries and promote collaborations, and how can they find chances to work in a U. S. laboratory. The fine points of our scientific debates were largely lost to them. In future meetings of this kind, perhaps more time should be spent on lectures on fundamental principles and less on recent discoveries and controversies.

Near the end of the meeting the author spent about two hours visiting the surface science laboratory headed by Renzo Rosei at the University of Trieste. The laboratory is brand new, with four rooms devoted to catalysis and low-energy electron diffraction, high-resolution electron energy loss spectroscopy, helium scattering, and molecular beam epitaxy. The equipment is of the latest design. When all laboratories are staffed and all instruments are on line, this research group can rival any surface science laboratory in productivity. In addition, a 2-GeV synchrotron light source with record high light intensity in the soft x-ray part of the electromagnetic spectrum will be completed in two years. This is a joint European project, backed by a consortium of government and industrial laboratories under the directorship of Rosei. The facility is especially suited to real-time studies of such complex problems as surface growth, catalysis, and biological reactions. The experimental group is supported by a group of theoretical physicists in Trieste devoted to computer simulation. Rosei received his Ph.D. in condensed matter physics in Rome and postdoctoral training in a wide range of optical measurements in the U. S., including one year at the Synchrotron Light Source in Stoughton, Wisconsin. He is a fine scientist and a capable administrator. The author has been personally acquainted with Rosei for over 20 years.

APPENDICES

- A. ITINERARY
- B. LIST OF PARTICIPANTS

APPENDIX A

ITINERARY

DATES	LOCATION	INDIVIDUALS CONTACTED	SUBJECT OF DISCUSSION
<u>1990</u>			
8/31-9/2	Travel en route from Oak Ridge, TN, to Trieste, Italy, via plane		
9/3-8	International Centre for Theoretical Physics, Trieste, Italy	M. P. Tosi, see List of Participants	Presentation of an invited lecture.
9/8-9	Travel en route from Trieste, Italy, to Oak Ridge, TN, via plane		

APPENDIX B

INTERNATIONAL ATOMIC ENERGY AGENCY
UNITED NATIONS EDUCATIONAL, SCIENTIFIC AND CULTURAL ORGANIZATION
INTERNATIONAL CENTRE FOR THEORETICAL PHYSICS
I.C.T.P., P.O. BOX 586, 34100 TRIESTE, ITALY, CABLE: CENTRATOM TRIESTE

Activity Code: 9011W015C

SMR Number: 524

WORKING PARTY ON
ELECTROCHEMISTRY - CONDENSED MATTER ASPECTS

27 August 1990 - 7 September 1990

PRELIMINARY LIST OF PARTICIPANTS

Total number of visitors for this activity = 62

* This list does not include scientists already present at the Centre or participating in the Research Workshop in Condensed Matter, Atomic and Molecular Physics.

Function Codes CD=Director
CL=Lecturer

CP=Participant
CT=Tutor

NC=Consultant
RE=Research

Status Codes FG=Group Associate
FH=Honorary Associate
FJ=Junior Associate
FR=Regular Associate
FS=Senior Associate

NA=SISSA/ICTP Agreement
NC=Adv.Comm.Member
NF=Affiliate
NG=Guest Scientist
NI=Italian Lab.Programme
NL=Guest Lecturer

NN=INFN/ICTP Agreement
NP=Microprocessor Lab.
NR=New Applicant
NS=Special Invited Guest
NV=Visiting Scientist

Updated: August 20, 1990

Name and Institute	Status	Nationality
--------------------	--------	-------------

FUNCTION: CD

Total Number in this Function = 1

1. KORNYSHEV Alexei A.

NG U.S.S.R.

Permanent Institute: Academy of Sciences of the Ussr
A.N. Frumkin Institute of Electrochemistry
Leninski Prospekt 31
V-71
Moscow 117071
U.S.S.R.

Name and Institute	Status	Nationality
FUNCTION: CL Total Number in this Function = 26		
2. BADIALI J.-P. Permanent Institute: Universite' de Paris VI (Pierre Et Marie Curie) Structure Et Reactivite Aux Interfaces Batiment F(74) 4 Place Jussieu Cedex 05 Paris 75230 France	NL	France
3. BOPP Philippe A. Permanent Institute: Rheinisch-Westfalische Technische Hochschule Institut Fuer Physikalische Chemie Templergraben 59 Aachen D-5100 Federal Republic of Germany	NL	France and Federal Republic of Germany
4. BREITER Manfred W. Permanent Institute: Vienna Technical University Institute of Technical Electrochemistry Getreidemarkt 9 Vienna A-1060 Austria	NL	Austria
5. FUNTIKOV Aleksander Permanent Institute: Academy of Sciences of the Ussr A.N. Frumkin Institute of Electrochemistry Leninskii Prospekt 31 V-71 Moscow 117071 U.S.S.R.	NL	U.S.S.R.
6. GERISCHER Heinz Permanent Institute: Fritz-Haber-Institut Der Max-Planck-Gesellschaft Faradayweg 4-6 Berlin 33 D-1000 Federal Republic of Germany	NL	Federal Republic of Germany

Name and Institute	Status	Nationality
7. GIMZEWSKI J. Permanent Institute: IBM Research Centre Zurich Research Laboratory Zurich Switzerland	NL	Switzerland
8. GUIDELLI Rolando Permanent Institute: Universita' degli Studi di Firenze Laboratorio di Elettrochimica Dipartimento di Chimica Via G. Capponi 9 Firenze 50121 Italy	NL	Italy
9. HUBBARD Arthur T. Permanent Institute: University of Cincinnati Department of Chemistry Ohio Cincinnati 45221-0172 U.S.A.	NL	U.S.A.
10. HYNES James Permanent Institute: University of Colorado Dept. Chemistry & Biochemistry Colorado Boulder 80309-0215 U.S.A.	NL	U.S.A.
11. KAZAR'NOV Vladimir Permanent Institute: Academy of Sciences of the Ussr A.N. Frumkin Institute of Electrochemistry Leninskii Prospekt 31 V-71 Moscow 117071 U.S.S.R.	NL	U.S.S.R.

Name and Institute	Status	Nationality
<p>12. KRISHTALIK Lev</p> <p>Permanent Institute: Academy of Sciences of the Ussr A.N. Frumkin Institute of Electrochemistry Leninskii Prospekt 31 V-71 Moscow 117071 U.S.S.R.</p>	NL	U.S.S.R.
<p>13. KUZNETSOV Alexander</p> <p>Permanent Institute: Academy of Sciences of the Ussr A.N. Frumkin Institute of Electrochemistry Leninskii Prospekt 31 V-71 Moscow 117071 U.S.S.R.</p>	NL	U.S.S.R.
<p>14. LIEBSCH Ansgar</p> <p>Permanent Institute: Kernforschungsanlage Julich GmbH Institut Fur Festkorperforschung Postfach 1913 Julich D-5170 Federal Republic of Germany</p>	NL	Federal Republic of Germany
<p>15. LIPKOWSKI Jacek</p> <p>Permanent Institute: University of Guelph Dept. Chemistry & Biochemistry Ontario Guelph N1G 2W1 Canada</p>	NL	Canada
<p>16. LIU Samuel H.</p> <p>Permanent Institute: Oak Ridge National Laboratory Solid State Division P.O. Box 2008 Oak Ridge TN 37831-6024 U.S.A.</p>	NL	U.S.A.

Name and Institute	Status	Nationality
17. PETTINGER Bruno Permanent Institute: Fritz-Haber-Institut Der Max-Planck-Gesellschaft Faradayweg 4-6 Berlin 33 D-1000 Federal Republic of Germany	NL	Federal Republic of Germany
18. PIAZZA Giuseppe Permanent Institute: Universita' degli Studi di Bologna Dipartimento di Chimica 'G. Ciamician' Via Selmi, 2 Bologna 40126 Italy	NL	Italy
19. PIRUG Gerhard Permanent Institute: Kernforschungsanlage Julich GmbH Institut Fur Grenzflächenforschung Und Vakuumphysik Postfach 1913 Julich D-5170 Federal Republic of Germany	NL	Federal Republic of Germany
20. SAPOVAL Bernard Permanent Institute: Ecole Polytechnique Laboratoire de Physique de La Matiere Condensee Route de Saclay F-91128 Cedex Palaiseau France	NL	France
21. SASS J. Permanent Institute: Fritz-Haber-Institut Der Max-Planck-Gesellschaft Faradayweg 4-6 Berlin 33 D-1000 Federal Republic of Germany	NL	Federal Republic of Germany

Name and Institute	Status	Nationality
<p>22. SCHMICKLER Wolfgang</p> <p>Permanent Institute: State University of New York At Stony Brook Department of Chemistry Long Island New York Stony Brook NY 11790 U.S.A.</p>	NL	Federal Republic of Germany
<p>23. STIMMING Ulrich</p> <p>Permanent Institute: Fritz-Haber-Institut Der Max-Planck-Gesellschaft Faradayweg 4-6 Berlin 33 D-1000 Federal Republic of Germany</p>	NL	Federal Republic of Germany
<p>24. ULSTRUP Jens</p> <p>Permanent Institute: the Technical University of Denmark Chemistry Department a Building 207 Lyngby DK-2800 Denmark</p>	NL	Denmark
<p>25. URBAKH Mikhail</p> <p>Permanent Institute: Academy of Sciences of the Ussr A.N. Frumkin Institute of Electrochemistry Leninskii Prospekt 31 V-71 Moscow 117071 U.S.S.R.</p>	NL	Israel
<p>26. VOROTYNTSEV M.A.</p> <p>Permanent Institute: Academy of Sciences of the Ussr A.N. Frumkin Institute of Electrochemistry Leninskii Prospekt 31 V-71 Moscow 117071 U.S.S.R.</p>	NL	U.S.S.R.

Name and Institute	Status	Nationality
27. WEAVER W.	NL	U.S.A.
Permanent Institute: Purdue University Department of Chemistry Chemistry Building Indiana West Lafayette 47907-3699 U.S.A.		

Name and Institute	Status	Nationality
FUNCTION: CP Total Number in this Function = 35		
28. AL-NAJAR Anis Abdulwahab	NR	Iraq
Permanent Institute: University of Basrah College of Science Department of Chemistry Basrah Iraq		
29. BORKOWSKA Zofia	NR	Poland
Permanent Institute: Polish Academy of Sciences Institute of Physical Chemistry Ul. Kasprzaka 44/52 Warsaw 01-224 Poland		
30. BRITO Pedro Cesar	NR	Argentina
Permanent Institute: Universidad Nacional de Tucuman Instituto de Fisica Fac.Ciencias Exact.Tecnologia Avda de La Independencia 1800 San Miguel de Tucuman RA-4000 Argentina		
31. CHAUDHARY Amjad Mohammad	NF	Pakistan
Permanent Institute: University of Engineering and Technology Department of Chemistry Lahore (31) Pakistan		
32. DELAVAR Mahmoud	NR	Islamic Republic of Iran
Permanent Institute: University of Birjand Department of Chemistry Birjand Islamic Republic of Iran		

Name and Institute	Status	Nationality
<p>33. DO Lien Ngoc</p> <p>Permanent Institute: Hanoi Institute of Nuclear Technology P.O.B. 5T-160 Nghia Do Tu Liem Hanoi Vietnam</p>	NR	Vietnam
<p>34. FU Jishi</p> <p>Permanent Institute: Beijing University (University of Peking) Department of Physics Faculty of Science Hai Dan Beijing 100871 People's Republic of China</p>	NR	People's Republic of China
<p>35. FUJIOKA Jorge</p> <p>Permanent Institute: Universidad Nacional Autonoma de Mexico Instituto de Fisica Apdo. Post. 20-364 Delegacion Alvaro Obregon Mexico City 01000 Mexico</p>	NR	Mexico
<p>36. GABOUZE Noureddine</p> <p>Permanent Institute: Haut Commissariat a La Recherche Udts 2. Bd Frantz Fanon B.P. 1017 Gare Algiers Algeria</p>	NR	Algeria
<p>37. GHEBREMEDHIN Michael Zaid</p> <p>Permanent Institute: Asmara University Department of Chemistry P.O. Box 1220 Asmara Ethiopia</p>	NF	Ethiopia

Name and Institute	Status	Nationality
<p>38. GOLOZAR Mohamad Ali</p> <p>Permanent Institute: Isfahan University of Technology D. of Mechanical Engineering Isfahan Islamic Republic of Iran</p>	NF	Islamic Republic of Iran
<p>39. HAI Vo Van</p> <p>Permanent Institute: National Centre For Scientific Research Hochiminh City Branch 1. Mac Dinh Chi Street 1Er Arrondissement Ho Chi Minh City Ho Chi Minh Vietnam</p>	NR	Vietnam
<p>40. HORANYI Tamas</p> <p>Permanent Institute: Semilab Semiconductor Physics Laboratory Rt. Foti Ut 56 P.O.B. 76 Budapest H-1047 Hungary</p>	NR	Hungary
<p>41. KAZMI Syed Arif</p> <p>Permanent Institute: University of Karachi Department of Chemistry University Road Karachi 75270 Pakistan</p>	NR	Pakistan
<p>42. KOWAL Andrzej</p> <p>Permanent Institute: Institute of Catalysis and Surface Chemistry Polish Academy of Sciences Ul. Niezapominajek Cracow 30239 Poland</p>	NR	Poland

Name and Institute	Status	Nationality
43. MEDINA-NOYOLA Magdaleno Permanent Institute: Universidad Autonoma de San Luis Potosi Instituto de Fisica Alvaro Obregon 64 San Luis Potosi 78000 Mexico	NF	Mexico
44. METIKOS-HUKOVIC Mirjana Permanent Institute: University of Zagreb Institute of Electrochemistry Dept. of Technology Savska C.16/1 Zagreb 41000 Yugoslavia	NR	Yugoslavia
45. MISHRA Naresh Chandra Permanent Institute: Utkal University Department of Physics Faculty of Science Vani Vihar Dist. Puri, Orissa Bhubaneswar 751 004 India	NR	India
46. MOHAJERI-MOGHAD Hamid Reza Permanent Institute: Ferdowsi University School of Science Department of Physics Faculty of Science Asrar Ave. Mashhad Islamic Republic of Iran	NF	Islamic Republic of Iran
47. MOORTHY Babu Sridharan Permanent Institute: Anna University Alagappa College of Technology Crystal Growth Centre Madras 600 025 India	NR	India

Name and Institute	Status	Nationality
<p>48. MOVASSAGHI Karim</p> <p>Permanent Institute: University of Isfahan Dept. of Chemistry Faculty of Sciences Isfahan Islamic Republic of Iran</p>	NR	Islamic Republic of Iran
<p>49. ODEH Issam</p> <p>Permanent Institute: Yarmouk University Department of Physics Faculty of Science P.O.B. 566 Irbid Jordan</p>	NF	Jordan
<p>50. RAHMAN Anisur Muhammed</p> <p>Permanent Institute: University of Rajshahi Department Applied Chemistry Rajshahi Bangladesh</p>	NI	Bangladesh
<p>51. REYES-MENA Arturo</p> <p>Permanent Institute: Centro de Investigacion Y de Estudios Avanzados del I.P.N. Departamento de Fisica Apartado Postal 14-740 Mexico City 07000 Mexico</p>	NF	Mexico
<p>52. ROSTAMI Abbas Ali</p> <p>Permanent Institute: University of Mazandaran P.O.Box 416 Babolsar Islamic Republic of Iran</p>	NR	Islamic Republic of Iran

Name and Institute	Status	Nationality
53. SEKKOU Kertit Permanent Institute: Ecole Normale Supérieure - Takaddoum Boite Postal 5118 Avenue Oued Akreuch Rabat Morocco	NR	Morocco
54. SHAWAGFEH Nabli Taleb Permanent Institute: University of Jordan Department of Mathematics Amman Jordan	NF	Jordan
55. SONG Kehui Permanent Institute: Beijing Institute of Technology Department of Applied Physics P.O. Box 327 Beijing 100081 People's Republic of China	NF	People's Republic of China
56. TRAORE Sekou Boukadary Permanent Institute: Ecole Normale Supérieure B.P. 241 Bamako Mali	NR	Mali
57. VESAGHI Mohammad Ali O.E. Permanent Institute: Sharif University of Technology Department of Physics Faculty of Science P.O. Box 11365-8639 Tehran Islamic Republic of Iran	NF	Islamic Republic of Iran

Name and Institute	Status	Nationality
58. WU Qiang Permanent Institute: University of Science and Technology of China Centre For Fundamental Physics 24 Jinzhai Road Anhui Hefei 230026 People's Republic of China	NR	People's Republic of China
59. YIANOULIS Panayiotis E. Permanent Institute: University of Patras Department of Physics Faculty of Science Patras 26110 Greece	NR	Greece
60. ZANJANIPOUR Mohammad Asghar Permanent Institute: Atomic Energy Organization of Iran P.O. Box 14155-1339 Tehran 14374 Islamic Republic of Iran	NR	Islamic Republic of Iran
61. ZELAYA-ANGEL Orlando Permanent Institute: Centro de Investigacion Y de Estudios Avanzados del I.P.N. Apartado Postal 14-740 Mexico City 07000 Mexico	NF	El Salvador
62. ZHENG Jiu-Ren Permanent Institute: University of Science and Technology of China Centre For Fundamental Physics 24 Jinzhai Road Anhui Hefei 230026 People's Republic of China	NF	People's Republic of China

END

DATE FILMED

10 / 22 / 90