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PUB-226

National Resource for Computation in Chemistry

BULLETIN

Lawrence Berkeley Laboratory
Building 50, Room 208
Berkeley, California 94720

Bulletin No. 4
Supplement
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PROPOSALS FUNDED

The NRCC is pleased to announce awards totaling \$119,385 for proposals funded from the second NRCC proposal review. Of the award total, \$103,280 (upwards of 165 hours of CDC-7600 time*) is for computation at the LBL Computer Center, \$13,105 (Ostlund) is to support studies at an institution other than the awardee's own, and \$3,000 (Fitch) is for work at the researcher's home institution. A brief description of the funded proposals follows.

Millard H. Alexander, Department of Chemistry, University of Maryland, "Theoretical Studies of Rotational Energy Transfer in Collisions between Polar Molecules." Quantum calculations of rotationally inelastic cross sections using a new decoupling approximation will be carried out on the HF-HF and LiH-HCl systems. (\$9,000 for 24 months)

Delos F. DeTar, Chemistry Department, Florida State University, "Applications of Molecular Mechanics to Large Molecules." Steric effects in enzyme-substrate interactions will be investigated by means of molecular mechanics, aiming at a quantitative estimation of the activation energies of enzyme-catalyzed reactions. (\$5,000 for 12 months)

Clifford E. Dykstra and Don Secrest, School of Chemical Sciences, University of Illinois, Urbana, "An Ion Triatomic Potential Surface Suitable for Vibrational Energy Transfer Calculation." An accurate potential energy surface for the system $Li^+ + CO_2$ will be generated and used for studies of vibrational energy transfer in the polyatomic system. (\$10,000 for 9 months)

D. E. Ellis, Department of Physics and Chemistry, and M. A. Ratner, Department of Chemistry, Northwestern University, "Application of Hartree-Fock-Slater Methods to Electronic Structure and Mobility Studies of Mixed-Valence Metal-Complex Linear Chain Conductors." Quantum chemical methods will be used to study the intermolecular delocalization in oligomeric species, specifically the nature of the conductivity process in linear-chain conductors built of planar metal complexes. (\$7,560 for 13 months)

Walter M. Fitch, University of Wisconsin, "Comparative Study of Protein and Nucleic Acid Structures." Computer-generated two-dimensional figures using conformal mapping techniques will be analyzed to obtain important features of tertiary and quaternary structures. (\$3,000 for 18 months.)

*Weekend and deferred rates are available and may increase one's capabilities up to fourfold.

PUB 226

Barbara J. Garrison and Nicholas Winograd, Department of Chemistry, Purdue University, "Determination of Surface Structure by Classical Trajectory Studies of Ion Bombardment Solids." The details of ion impact phenomena in solids will be investigated using classical trajectory techniques with the goal of obtaining information about the structure of atoms and molecules on surfaces. (\$10,000 for 12 months)

Thomas George, Department of Chemistry, University of Rochester, "Computational Studies of Laser-Assisted Molecular Rate Processes." Two studies are proposed. The first is a semiclassical calculation on the reaction $F(^2P_{3/2}) + H_2 \rightarrow HF + H$ in the presence of the 1.06 μm light of the Nd:glass laser. The second is an investigation of the role of photon angular momentum in a fully quantum mechanical treatment of molecular collisions occurring in a laser field. (\$5,000 for 15 months)

Peter A. Kollman, University of California, San Francisco, "Modeling Studies for Large Molecule-Small Molecule Interactions." A general computer program to model large molecule-small molecule interactions and empirical potential functions for the study of nucleic acid conformations and interactions will be developed. (\$8,320 for 18 months)

I. D. Kuntz and Gordon Crippen, Department of Pharmaceutical Chemistry, University of California, San Francisco, "Application of Distance Geometry to Conformational Analysis of Medium-Sized Molecules." The mathematical techniques of distance geometry will be used in a new approach to the problem of finding low energy conformations of medium-sized molecules (50 to 500 atoms). (\$8,500 for 15 months)

Vincent McKoy, Laboratory of Chemical Physics, California Institute of Technology, "Electron-Molecular Ion Scattering Cross Sections." A new discrete basis set approach will be developed for the solution of the electron-molecular-ion scattering problem. (\$5,000 for 12 months)

Neil S. Ostlund, Department of Chemistry, University of Arkansas, "Design and Implementation of Parallel Algorithms for Quantum Chemical Calculations." Design of parallel algorithms for the solving of Roothaan's equations on a large multi-microprocessor computer system (CM*) built by the Computer Science Department at Carnegie Mellon University. (\$13,105 for 6 months)

William P. Reinhardt, Department of Chemistry, University of Colorado, "Atoms in Intense Fields." Multiphoton ionization processes of Cs and atomic H, along with the structure of atoms in laser fields crossed with a dc field will be studied. (\$3,000 for 18 months)

Stuart A. Rice, The James Franck Institute, University of Chicago, "Computer Simulation of the Surface of a Liquid Metal." The study will use a generalization of the Monte Carlo technique to simulate the properties of a liquid metal surface. (\$8,000 for 12 months)

K. T. Tang, Physics Department, Pacific Lutheran University, "Quantum Theory of Reactive and Inelastic Molecular Scattering." The development and application of polarized target coupling method for atom-molecule reactive scattering will be carried out. (\$7,500 for 12 months)

David R. Yarkony, Chemistry Department, Johns Hopkins University and Charles W. Bauschlicher, Jr., NASA Langley Research Center, "Theoretical Aspects of Electronic Energy Transfer Processes in Reactions of the Form $Me + O-A \rightarrow MeO + A$." *Ab initio* electronic structure techniques will be used to study the above reactions in which the electronically excited metal oxide product is a laser candidate. (\$16,400 for 12 months)

CALL FOR PROPOSALS

In the coming year, the NRCC will have two calls for submission of proposals. The deadlines for receipt of proposals are January 15, 1979, and July 15, 1979. Awards will be announced for the earlier call in mid-April 1979, and for the later one in mid-October 1979.

Proposals are sought for an allotment of computer time to be used at the LBL Computer Center (or elsewhere upon approval of both the NRCC Program Committee and NRCC Policy Board). Proposals may be from any field of chemistry and should promote the development of chemistry through: the advancement of computational methods; the innovative application of existing methods to problems in some frontier area of chemistry; the study of problems of significant scientific merit that cannot be carried out in the proposer's institution due to lack of large-scale computational facilities; the resolution of intradisciplinary computational methodology issues; and the development of interdisciplinary approaches to forefront problems in chemistry.

The list of awards from the second review of 1979 might lead to the impression that only proposals requiring modest amounts of computer time will be funded. On the contrary, with each round of proposals, the NRCC is attempting to increase the funds available for awards. With the prospect of increased funds, the NRCC Program Committee wishes to emphasize the importance of receiving proposals of broad scope and effort. In addition, it should be noted that the NRCC scientific staff can assist as an information resource, and in collaborative efforts where appropriate. Inquiries concerning the latter should be forwarded to the NRCC Director, Dr. William A. Lester, Jr.

Directions for proposal preparation are appended. The LBL Computer system is a complex consisting of a CDC-7600, CDC-6600 and CDC-6400. Further information on the LBL computer system, its rate structure, and details on using it may be obtained by writing to the NRCC, Attention: User Coordinator.

DIRECTIONS FOR PROPOSAL PREPARATION

The NRCC has established the following guidelines for the submission of proposals which supersede those previously provided.

COVER PAGE

The following information should appear on the cover page:

1. Name of principal investigator(s) submitting proposal.
2. Name of submitting organization (including department).
3. Address (including building and room where appropriate).
4. Telephone number.
5. Title of proposed research.
6. Hours of CDC-7600 computing time. Desired level: _____ hours.
Threshold level: _____ hours.
7. Proposed starting date.
8. Proposed duration of the research.
9. Previous anniversary date and account number (for renewal or continuing award request).

ABSTRACT

A brief summary of the proposed research, including significance to science and impact for the NRCC.

NARRATIVE PROPOSAL

The narrative should be no more than 10 double-spaced typewritten pages and include the following information:

1. A description of the work being proposed, including the objectives, significance, and nature of the calculations.
2. A general plan for achieving these objectives, including an explanation of the methods to be used.
3. Relation of the proposed work to the current status of the topic addressed.
4. Outline (with pertinent references) of what has been done on the topic to date.
5. Explanation of how this research will advance understanding in the subject area of chemistry.
6. Justification of requested hours of computer time.
7. A bibliography of pertinent literature.

STATEMENT ON BUDGET

The financial statement section should include the following information:

1. Detailed line item budget for the grant monies required, including computer costs, travel costs and communication costs (if any).
2. Other agencies, if any, to which the proposal will be submitted.
3. All current support: title of project, funding period of award(s), agency and annual budget levels.
4. Other proposals (including renewal applications) which are currently pending (including DOE and NSF).

STATEMENT OF STAFFING

The statement of staffing should include the following documentation:

1. List of all collaborators who will be computing on the research outlined in the proposals (include names, titles, and telephone numbers).
2. Curriculum vitae of the principal investigator(s).
3. Principal publications of other senior personnel during the past five years on the subject matter covered by the proposal.

STATEMENT ON COMPUTER CAPABILITIES

1. Have you ever computed at LBL before? If not, skip 2-4, and answer 5 and 6.
2. If so, are you currently connected to the LBL computer system?
3. What is your access code (account number)?

4. What type of equipment is currently available to you for connection with the LBL Computer Center?

(a) RECC Terminal (make_____ model_____)

(b) RJE (make_____ model_____)

(c) Other (make_____ model_____)

5. Briefly describe the available equipment, policies, and capabilities of the computer center at your institution.

6. Briefly describe the hardware and communications software available, if any, for remote access to the LBL computer center.

STATEMENT ON COMMUNICATION AVAILABILITY

1. LBL has provided communication systems (TYMNET, ARPANET and FTS) for toll-free access to the LBL computers for interactive (RECC) calculations. If you are planning to compute via the Remote Batch Entry System (RJE), have you made provisions, either in the proposal or elsewhere, for communication costs? If so, please explain in detail.

2. Is your computer terminal connected to any other leased phone line system? If so, what kind?

3. Do you have a teletype (TWX) machine available to you? If so, what is the phone number of the machine?

4. Do you have a telecopier available to you? If so, list the make, speeds, type (automatic or manual), machine telephone number, and confirmation telephone number.

LAWRENCE BERKELEY LABORATORY
COMPUTER CENTER RATE SCHEDULE

October 1, 1978

(1) Rates \$0.0475 per Accounting Unit (AU) + LBL Overhead

Note: This approximates \$250 per hour for the CDC 6600 or \$1000 per hour for the CDC 7600. There is no exact hourly rate available, but for estimation purposes these rates approximate charges made by a typical job's use of the facilities.

(2) Accounting Algorithm

(a) Accounting Units (AUs)

$AUs = p*CU + J$ on weekdays

$= 0.5 * ((P*CU) + J)$ on weekends and holidays

where $P = 2.0$ for rush jobs

1.0 for normal jobs

0.75 for deferred jobs

0.5 on weekends or holidays

$J = 10$ for CDC 7600 job and 2 for CDC 6600 job

(b) Computing Units (CUs)

7600 CUs = $3*(CP+SS) + 0.5*BLD + ITO + STAGING$

6000 CUs = $(M*CP + 20*KMR)*(1 + CM/32768) + (10*MT) + TTY$

where CP = CPU time in seconds used by the job

SS = CPU time for 7600 jobs' systems tasks

BLD = LCM buffer loads

ITO = Interference to others factor

$= (4*MAX(1.2*CP, BLD/3) - (3*CP + BLD/2)*LCM/400000)_{10}$

LCM = instantaneous LCM field length

MAX = algebraic maximum

STAGING = staging job's CUs on the 6000 computers

$M = 0.7$ for 6600, 0.4 for 6400

KMR = number of monitor requests for system services (in thousands)

CM = instantaneous field length

MT = number of magnetic tapes hung

TTY = teletype CUs if a teletype is connected to the job:

midnight to 6 AM: 0.25 CU/connect minute

6 AM to 10 AM: 0.50 "

10 AM to 6 PM: 1.00 "

6 PM to midnight: 0.50 "

(3) Supplies and Handling Charges

0.10 AU per printed page

0.05 AU per punch card

5.00 AU per 105mm fiche

0.20 AU per 35mm frame

0.10 AU per 16mm frame

1.00 AU per 20 inches of Calcomp plot paper or per 1 minute of plotting time

5.00 AUs per queued output file processed on weekdays

2.50 AUs per queued output file processed on weekends or holidays

(4) Remote Use Charges

Line Capacity

2000 baud

4800 baud

7200 baud

9600 baud

Dial Up Line (Bell System)

3.50/hr + LBL overhead

5.00/hr + LBL overhead

not available

not available

Dedicated Line

\$150/month + LBL overhead

200/month + LBL overhead

275/month + LBL overhead

300/month + LBL overhead

(5) LBL Overhead

Charges described above are all subject to the current Laboratory overhead charge.

This is estimated at 40½% for the fiscal year ending 9/30/79 but is subject to monthly fluctuations.

(6) Full-Cost Recovery Including Depreciation and DOE-Added Factor

The recent Comptroller General's decision, B-136318 (1-21-77), requires services rendered under the Economy Act be reimbursed on the basis of actual cost plus all significant indirect costs.

Under this policy, the Laboratory must charge other federally-funded users at the DOE full-cost recovery rate including depreciation and the DOE-added factor unless the work qualifies as DOE-related and an exception is approved. Depreciation and the added factor will add approximately 20% to all applicable costs outlined above.

PUB-226

NRCC

Lawrence Berkeley Laboratory

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For Reference

Not to be taken from this room