American Chemical Society

National Awards Nomination Packet

ACS Award in Theoretical Chemistry:2018
for: James Anderson

Received: 11/01/2016 *Cycle Year: 1*

"For outstanding contributions to quantum chemistry, chemical kinetics and molecular dynamics"

NOMINATOR:

William Lester
Univ of California
Chem Dept
Berkeley, CA 94720-1460
UNITED STATES

Tel: (510)635-9782
Fax: (510)642-1088
Email: walester@berkeley.eduXXX

- Have you discussed this award nomination with the nominee? *Yes*

NOMINEE:

James Anderson
Penn State Univ
104 Chemistry Bldg
University Park, PA 16802-4615
UNITED STATES

Tel: (814)237-8442
Email: jba@psu.eduXXX

ACS Current Member: Yes
Years of Service: 60
Date of birth: 01/01/1935
Present Position: Evan Pugh Professor of Chemistry and Physics
Industry: Academia

CODE OF CONDUCT:

- To the best of my knowledge, including past and present circumstances, the nominee:
  1. Employs and requires good safety protocols and practices in his/her laboratory and/or work environment;
  2. Upholds the highest ethical standards in his/her laboratory and/or work environment; and
  3. Otherwise engages in conduct that is consistent with both the objects of the American Chemical Society as stated in Article II Section 1 of its Constitution and the Chemical Professional Code of Conduct.

Code of Conduct Answer: *Yes*

SUPPORTER 1

Anne McCoy
University of Washington
Po Box 351700
Seattle, WA 98195-1700
UNITED STATES

Tel: (202)543-7464
Email: abmccoy@uw.eduXXX

Recommendation:

Dear Award Committee:I write to nominate Professor James B. Anderson, Department of Chemistry, Penn State University for the 2017 ACS Award in Theoretical Chemistry. Professor Anderson has made key contributions in several areas of theoretical chemistry: in reaction kinetics and molecular dynamics, in the 'rare-event' approach to chemical reactions, in quantum Monte Carlo methods (QMC), and in direct Monte Carlo simulation of reaction systems. I discuss below three of these areas that best illustrate innovative research and advances in theoretical methodology and have assisted in new discoveries about chemical systems. Others are included in a short list of his most important publications that accompany the nomination. Professor Andersons first theoretical studies were in the area of nozzle-source molecular beams (supersonic beams). This research contributed to success in generating molecular beams of high energies, high fluxes, and narrow velocity distributions that have been especially useful in studies of reaction dynamics.Andersons experiments with supersonic beams for the reaction HI HI H2 I2 led him to early investigations with classical trajectory calculations. He carried out the first calculations of the F-H-H system with a study of the energy requirements for the reaction H HF H2 F and followed this with calculations of F H2 HF H, a reaction of special interest in theoretical chemistry because it is one of the simplest examples of an exothermic chemical reaction. Trajectory calculations for the reaction HI HI , a rare event, led to his research on the prediction of rare events in molecular dynamics by sampling trajectories crossing a surface in phase space. The method reduced the computational effort for such calculations by five orders of magnitude. Initially called variational theory of reaction rate by Keck (1960) and subsequently combined phase-space trajectory method by Anderson (1973), it is now often called the reactive flux method after Miller et al. (1980). Anderson extended Kecks original method and defended it against a number of critics. He wrote an extensive review in 1995 describing applications to that date. The earliest of these were three- and four-body reactions. The first application to condensed matter was by Bennett (1980), the first to protein folding was by McCammon and Karplus (1980), and the first for enzyme reactions was by Neria and Karplus (1997). Both Karplus and Warshel have been major users of the approach. The method is now the standard by which Kramers theory, Grote-Hynes theory, and related methods for molecular dynamics in solution are judged. Professor Anderson pioneered in the development of the QMC method of simulating the Schrdinger equation. His 1975-76 papers were the first to describe applications of random walk methods to polyatomic systems and many-electron systems. (The term Quantum Monte Carlo was coined by McDowell and Doll in 1981.) With exact QMC, Anderson was the first to reach an uncertainty of one microhartree for a polyatomic species (H3) and an uncertainty of one calorie for linear H-H-H, the saddle point of the hydrogen exchange reaction. Today, QMC methods are often the preferred choice for high accuracy for the electronic structure of molecules, molecules in solution, the electron gas, clusters of various types, solid materials, vibrating molecules, and many other classes of systems. Andersons recent book (2007) describes the origins, development and applications of the method. A recent search (2016) of the literature reveals more than 5000 papers with the words quantum chemistry by random walk, diffusion Monte Carlo, or quantum Monte Carlo in the title or abstract. The QMC method has the advantage of scaling with only the third power of the size of a system, while other high-level methods scale with the fifth or sixth power. At the level of, for example, carbon-20, the major competitor for fixed-node QMC is the CCSD(T) variant of coupled-cluster theory. It is clear that QMC is now well established in quantum chemistry along with SCF, MP2, MP4, CISD, CCSD, and DFT. QMC has often been cited as the gold standard for electronic structure calculatons, but recent QMC calculations (2016) by several authors using multi-term CI for locating nodes perform even better. Anderson has made a remarkable series of contributions to chemistry, in general, and to theoretical chemistry, specifically. I trust that the value of these contributions will be recognized with the selection of James Anderson for the ACS Award in Theoretical Chemistry for 2018. Sincerely yours,William A. Lester, Jr.

James Bernhard Anderson **September 2016**
Evan Pugh Professor of Chemistry and Physics
Pennsylvania State University

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University Park, Pennsylvania, USA 16802

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email: jba@psu.edu website: www.personal.psu.edu/jba/

Home Address: 426 Ridge Avenue
State College, PA 16803
Telephone: (814) 237-8442

Professional Experience:

1974 - present Associate Professor/Professor/Evan Pugh Professor
Department of Chemistry
The Pennsylvania State University

2002 – present Evan Pugh Professor
Department of Physics
The Pennsylvania State University

2001 – 2009 Director, Consortium for Education in Many-Body Applications

1968 - 74 Associate Professor
Department of Engineering and Applied Science
Yale University

1964 - 68 Assistant Professor
Department of Chemical Engineering
Princeton University

1964 Visiting Lecturer (part-time)
Department of Chemical Engineering
Rutgers University

1963 - 64 Postdoctoral Research Associate
Department of Chemical Engineering
Princeton University

1958 - 60 Petrochemical Research & Development Engineer
Shell Chemical Company
Deer Park, Texa

Education:

The Pennsylvania State University, 1953 - 57
B.S., Chemical Engineering, 1957

University of Illinois, 1957 - 58
Major Professor: Max S. Peters
Thesis: Kinetics of the Aldol Condensation
M.S., Chemical Engineering, 1958

Princeton University, 1960 - 63
Major Professor: Michel Boudart
Thesis: Sticking Probability of Oxygen on Germanium
M.A., Chemical Engineering, 1962
Ph.D., Chemical Engineering, 1963

Professional Society Membership:

American Chemical Society
American Physical Society
American Association for the Advancement of Science

Consulting:

Lawrence Livermore National Laboratory
Sandia National Laboratory
Exxon-Mobil Research and Engineering Company

Honors:

Bausch and Lomb Award
Evan Pugh Medal (Silver)
Evan Pugh Medal (Gold)
National Science Foundation Graduate Fellowship
Fellow of the American Physical Society
Fellow of the American Association for the Advancement of Science
Faculty Scholar Medal
Senior Research Award, Alexander von Humboldt Foundation, Bonn, Germany

Visiting Professorships:

Department of Theoretical and Organic Chemistry, Cambridge University
January - June, 1985

Department of Chemistry, University of Milan
October, 1992

Department of Physics, University of Kaiserslautern
January - July, 1994

Department of Chemistry, Göttingen, Germany
Summer, 1995

Department of Physical Chemistry, Free University of Berlin
Fall, 2000

Department of Chemistry, RWTH – Aachen University
Fall, 2007

James B. Anderson Short 20-item Publications List October 2016
see also website: www.personal.psu.edu/jba/

Molecular Beams

1. J. B. Anderson and J. B. Fenn, *Velocity Distributions in Molecular Beams from Nozzle Sources*, Phys. Fluids 8, 780-787 (1965).

2.. N. Abuaf, J. B. Anderson, R. P. Andres, J. B. Fenn and D. G. H. Marsden, *Molecular Beams with Energies Above One Electron Volt*, Science 155, 997-999 (1967).

3. S. B. Jaffe and J. B. Anderson, *Molecular Beam Study of the Hydrogen Iodide Reaction* , J. Chem. Phys. 51, 1057 (1969).

4. J. B. Anderson and P. Davidovits, *Isotope Separation in Seeded Beams*, Science 187, 642 (1975).

Classical Trajectory Calculations

5. J. B. Anderson, *Energy Requirements for Chemical Reaction:* $H + HF \rightarrow H_2 + F$, J. Chem. Phys. 52, 3849-3850 (1970).

6. R. L. Jaffe and J. B. Anderson, *Classical Trajectory Analysis of the Reaction* $F + H_2 \rightarrow HF + H$, J. Chem. Phys. 54, 2224-2236 (1971).

Rare Event Theory aka Reactive Flux

7.. J. B. Anderson, *Statistical Theories of Chemical Reactions. Distributions in the Transition Region*, J. Chem. Phys. 58, 4684 (1973).

8. R. L. Jaffe, J. M. Henry and J. B. Anderson, *Variational Theory of Reaction Rates: Application to* $F + H_2 \Leftrightarrow HF + H$, J. Chem. Phys. 59, 1128 (1973).

9. J. B. Anderson, *A Test of the Validity of the Combined Phase-Space/Trajectory Method*, J. Chem. Phys. 62, 2446 (1975).

10. R. L. Jaffe, J. M. Henry and J. B. Anderson, *Molecular Dynamics of the Hydrogen Iodide and Hydrogen-Iodine Exchange Reactions*, J. Am. Chem. Soc. 98, 1140-1155 (1976).

11. J. B. Anderson, *Predicting Rare Events in Molecular Dynamics*, Advances in Chemical Physics 91, 381 (1995).

Quantum Monte Carlo

12. J. B. Anderson, *A Random-Walk Simulation of the Schrödinger Equation:* H_3^+ , J. Chem. Phys. 63, 1499 (1975).

13. J. B. Anderson, *Quantum Chemistry by Random Walk:* $H\ ^2P$, $H_3^+\ D_{3h}\ ^1A_1$, H_2 , $Be\ ^1S$,

J. Chem. Phys. 65, 4121-4127 (1976).

14. J. B. Anderson, *Quantum Chemistry by Random Walk: H_4 Square*, International Journal of Quantum Chemistry 15, 109-120 (1979).

15. D. R. Garmer and J. B. Anderson, *Quantum Chemistry by Random Walk: Methane*, J. Chem. Phys. 86, 4025 (1987).

16. D. L. Diedrich and J. B. Anderson, *An Accurate Monte Carlo Calculation of the Barrier Height for the Reaction* $H + H_2 \rightarrow H_2 + H$, Science 258, 786 (1992).

17. J. B. Anderson, C. A. Traynor, and B. M. Boghosian, *An Exact Quantum Monte Carlo Calculation of the Helium-Helium Intermolecular Potential*, J. Chem. Phys. 99, 345 (1993).

18. S. Sokolova, A. Lüechow, and J. B. Anderson, *Energetics of Carbon Clusters C_{20} from All-Electron Quantum Monte Carlo Calculations*, Chem. Phys. Lett. 323, 229-233 (2000).

19. J. B. Anderson, *Quantum Monte Carlo: Origins, Development, Applications*, Oxford University Press, 2007. (January 2007, 212 pp.)

20. J. B. Anderson, *"Exact" Quantum Monte Carlo Calculations of the Barrier for the $H + H_2$ Reaction at the Sub-microhartree Level,* J. Chem. Phys. 144, 166101 (2016).

UNIVERSITY of WASHINGTON
DEPARTMENT OF CHEMISTRY

Anne B. McCoy
Professor

October 25, 2016

Dear Members of the Selection Committee,

It is with great pleasure that I write this letter in support of Professor William Lester's nomination of Professor James B. Anderson for the ACS Award in Theoretical Chemistry. As Bill outlined in his nomination letter, Professor Anderson's contributions are both broad and important, ranging from early studies on molecular beams with John Fenn to studies of chemical reaction dynamics and kinetics and into electronic structure theory. It is hard to think of many theorists who have made such a range of important and early contributions in theoretical chemistry.

The area of Anderson's contributions that I am most familiar with has been his work in the development of and implementations of quantum Monte Carlo. This approach, which was originally outlined in a pair of papers that were published in 1975 and 1976, comes from a recognition that the stationary state solution to the Schrodinger equation can be obtained through random walk methods, allowing for the application of statistical approaches to the evaluation of energies and wave functions.

The articulation of this approach coincided with the availability of increasingly powerful computers and computer architectures. Unlike many of the other methods that have been developed for studying quantum mechanical systems quantum Monte Carlo approaches have been applied to detailed studies of relatively small systems as well as quite large systems. These approaches also translate well from electronic structure problems to studies of molecular vibrations, particularly for molecular systems that undergo large amplitude excursions from the equilibrium structure at relatively low energies. Such problems are very challenging to investigate by basis set-based approaches, but are very amenable to these Monte Carlo approaches.

The breadth of applications is attributed to the combination of relative simplicity and complete generality of the underlying theory. It also comes from the highly favorable scaling of quantum Monte Carlo approaches, relative to other quantum chemical approaches. In addition, the quantum Monte Carlo algorithms are well-suited for the massively parallel environments in contemporary computing environments. Based on this, quantum Monte Carlo approaches are receiving increasing interest in the community, for studying a diverse range of problems.

Such early recognition of important algorithmic advances and problems in theoretical chemistry has been a hallmark of Professor Anderson's career. It is for the combination of depth and breadth important contributions to the field that I provide my strongest support of Professor Lester's nomination of James Anderson for the ACS Award in Theoretical Chemistry.

Sincerely,

Anne B. McCoy
Professor of Chemistry
Deputy Editor, Journal of Physical Chemistry A