WILLIAM A. GODDARD, III
California Institute of Technology:
Charles and Mary Ferkel Professor of Chemistry, Materials Science, and Applied Physics
Director of Materials and Process Simulation Center (MSC)
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Research Profile

Goddard has been a pioneer in developing methods for quantum mechanics (QM), force fields (FF), reactive dynamics (ReaxFF RD), electron dynamics (eFF), molecular dynamics (MD), and Monte Carlo (MC) predictions on chemical, catalytic, and biochemical materials systems and is actively involved in applying these methods to ceramics, semiconductors, superconductors, thermoelectrics, metal alloys, polymers, proteins, nuclei acids, Pharma ligands, nanotechnology, and energetic materials. A particular focus has been to determine the detailed reaction mechanisms underlying heterogeneous and homogeneous catalysts, including electrocatalysis. The goal of the Goddard research has been to develop the methods sufficiently accurate that the need for experimental validation can be severely restricted to the predicted best systems and sufficiently efficient that they can be applied to realistic systems with millions of atoms (now referred to as Materials Genomics). This required improving the QM (particularly for van der Waals binding and band gaps) while improving the methods for matching the FF to QM for describing large scale reactive systems. He uses hierarchical approaches (multiscale, multiparadigm) to couple between the electronic states of QM with dynamics of macroscale systems, enabling first-principles based accuracy of realistic systems (millions of atoms, millisecond time scales). A recent advance adaptive accelerated ReaxFF Reactive Dynamics (aARRDyn) demonstrated similarly of 9 minutes of hydrogen oxidation reactions using 1.3 million time steps. The Materials and Process Simulation Center (MSC) that he founded and directs, has a critical mass of expertise in all these areas to improve the methods and apply simulations to problems of interest to industry and government labs.

Previous Professional Positions (all at Caltech):

2001-present	Charles and Mary Ferkel Professor of Chemistry, Materials Science, Appl. Phys.
1990-present	Director of Materials and Process Simulation Center (MSC)
1992-1997	Director of NSF Grand Challenge Applications Group at Caltech
1984-2001	Charles and Mary Ferkel Professor of Chemistry and Applied Physics
1984-1990	Director of NSF Materials Research Group at Caltech
1978-1984	Professor of Chemistry and Applied Physics
1967-1978	Assistant, Associate, and Full Professor of Theoretical Chemistry
Nov. 1964-Dec. 1966	Alfred A. Noyes Research Fellow of Chemistry

Education:

Ph.D. Engineering Science (minor physics), California Institute of Technology, 1965 (Oct. 1964)
BS Engineering (Highest Honors), University of California, Los Angeles, 1960.

Selected Awards and Honors (since 1984)

- Elected Member of National Academy of Science (1984)
- Elected Member of International Academy of Quantum Molecular Science (1988)

- Elected Fellow of American Physical Society (1988)
- Winner American Chemical Society Award for Computers in Chemistry (1988)
- Awarded Feynman Prize for Nanotechnology Theory (1999)
- Named ISI Highly Cited Chemist for 2001 (http://isihighlycited.com)
- Winner 2002 Prize Computational Nanotechnology Design (Inst. Molecular Manufacturing)
- Awarded American Chemical Society Award for Theoretical Chemistry (2007)
- Elected Fellow of the Royal Society Chemistry (2008)
- Awarded NASA Space Sciences Award for Space Shuttle Sensor (2009)
- Awarded NASA Space Sciences Award for polymer films (2012)
- World Class University Professor in the Energy, Environment, Water, Sustainability (EEWS) Graduate School, at the Korea Advanced Institute of Science and Technology (KAIST), Daejeon, Korea (2009-2013)
- Award for Distinguished Scientific Achievement in Catalysis 7th World Congress Oxidation Catalysis (2013)
- Named ISI Highly Cited Chemist for 2014 (http://isihighlycited.com)
- IISc-DST Centenary Chair Professor at the Indian Institute of Science, Bangalore India, 2015
- Named ISI Highly Cited Chemist for 2015 (http://isihighlycited.com)

Selected Recent Research publications: total over 1155, (H index = 126, I-10 index 933)
https://scholar.google.com/citations?user=yMZlErUAAAAJ&hl=en
http://www.wag.caltech.edu/publications/papers/

1. **Quantum Mechanical and Experimental Validation that Cyclobis(paraquat-p-phenylene) Forms a 1:1 Inclusion Complex with Tetrathiafulvalene;** Hartlieb KJ; Liu WG; Fahrenbach AC; Blackburn AK; Frasconi M; Hafezi N; Dey SK; Sarjeant AA; Stern CL; Goddard WA & Stoddart JF; Chem. Eur. J., **1** (22): 2736-2745 (**2016**) wag1154
2. **Oligorotaxane Radicals under Orders;** Wang Y; Frasconi M; Liu WG; Sun JL; Wu YL; Nassar MS; Botros YY; Goddard WA; Wasielewski MR & Stoddart JF; ACS Cent. Sci., Article ASAP, DOI: 10.1021/acscentsci.5b00377 (**2016**) wag1153
3. **Non-Radiative Plasmon Decay and Hot Carrier Dynamics: Effects of Phonons, Surfaces and Geometry;** Brown AM; Sundararaman R; Narang P; Goddard WA & Atwater HA; ACS Nano, DOI: 10.1021/acsnano.5b06199, (**2015**) wag1152
4. **First-principles Modeling of Ni 4 M (M = Co, Fe and Mn) Alloys as Solid Oxide Fuel Cell Anode Catalyst for Methane Reforming;** Tsai HC; Morozov SI; Yu TH; Merinov BV & Goddard WA; J. Phys. Chem. C, DOI: 10.1021/acs.jpcc.5b06847 (**2015**) wag1151
5. **Mechanistic Explanation of the pH Dependence and Onset Potentials for Hydrocarbon Products from Electrochemical Reduction of CO on Cu(111);** Xiao H; Cheng T; Goddard WA & Sundararaman R; J. Am. Chem. Soc., DOI: 10.1021/jacs.5b11390 (**2015**) wag1149
6. **Reaction Mechanism for Ammonia Activation in the Selective Ammoxidation of Propene on Bismuth Molybdates;** Pudar S & Goddard WA; J. Phys. Chem. C, **119** (49): 27370-27381 (**2015**) wag1148
7. **Holey Graphene as a Weed Barrier for Molecules;** Gethers ML; Thomas JC; Jiang S; Weiss NO; Duan X; Goddard, WA & Weiss, PS; ACS Nano, **9** (11): 10909-10915 (**2015**) wag1147
8. **Free Energy Barriers and Reaction Mechanisms for the Electrochemical Reduction of CO on the Cu(100) Surface Including Multiple Layers of Explicit Solvent at pH 0;** Cheng T; Xiao H & Goddard WA; J Phys. Chem. Lett., DOI:10.1021/acs.jpclett.5b02247 (**2015**) wag1145

9. **Computational Prediction and Biochemical Analyses of New Inverse Agonists for the CB1 Receptor;** Scott C; Ahn KH; Graf ST; Goddard WA; Kendall DA & Abrol R; J Chem. Inf. Model., DOI:10.1021/acs.jcim.5b00581 (**2015**) wag1144
10. **Prediction of the Chapman-Jouguet Chemical Equilibrium State in a Detonation Wave from First Principles Based Reactive Molecular Dynamics;** Guo D; Zybin SV; An Q; Goddard WA & Huang FL; Phys. Chem. Chem. Phys., **1** (18): 2015-2022 DOI: 10.1039/C5CP04516A (**2016**) wag1142
11. **Improved Ductility of Boron Carbide by Microalloying with Boron Suboxide;** Tang B; An Q & Goddard WA; J. Phys. Chem. C, **119** (43): 24649-24656 (**2015**) wag1134
12. **Annealing kinetics of electrodeposited lithium dendrites;** Aryanfar A; Cheng T; Colussi AJ; Merinov BV; Goddard WA & Hoffmann MR; J. Chem. Phys., **143** (10): 134701 http://dx.doi.org/10.1063/1.4930014 (**2015**) wag1133
13. **Fractal atomic-level percolation in metallic glasses;** Chen DZ; Shi CY; An Q; Zeng Q; Mao WL; Goddard WA & Greer JR; Science, **349** (6254): 1306-1310 DOI: 10.1126/science.aab1233 (**2015**) wag1132
14. **Accurate ab initio Quantum Mechanics of Bi2Se3 and Bi2Te3 Topological Insulator Surfaces;** Crowley JM; Tahir-Kheli J & Goddard WA; J. Phys. Chem. Lett., **6** (19): 3792-3796 (**2015**) wag1130
15. **In Silico Design of Highly Selective Mo-V-Te-Nb-O Mixed Metal Oxide Catalysts for Ammoxidation and Oxidative Dehydrogenation of Propane and Ethane;** Mu-Jeng Cheng and William A Goddard III. J. Am. Chem. Soc. **137** (41): 13224-13227 (**2015**) wag1120
16. **Atomistic Origin of Brittle Failure of Boron Carbide from Large-Scale Reactive Dynamics Simulations: Suggestions toward Improved Ductility;** An Q & Goddard WA Phys. Rev. Lett., **115** (10): 105501 (**2015**) wag1128

Books

1. Handbook of Nanoscience, Engineering, and Technology, Third Edition; William A Goddard III, Donald W. Brenner, Sergey E. Lyshevski, and Gerald J. Iafrate CRC Press Taylor and Francis Group, 2012; Print ISBN: 978-1-4398-6015-1; eBook ISBN: 978-1-4398-6016-8
2. Metalloproteins: Theory, Calculations, and Experiments. Art E. Cho and William A Goddard III, CRC Press Taylor and Francis Group, 2015.ISBN: 13:978-1-4398-1318-S

Other Professional Activities:

Consultant (at various times): General Electric, General Motors, Shell Development, Imperial Chemical Industry, BP, Exxon, Chevron, SOHIO, Dow Chemical, AT&T Bell Labs, Union Carbide, Celanese, Allied Signal, UOP, 3M, Proctor and Gamble, Dow Corning, Nissan, MSI (Accelrys), Schrödinger, Eidogen, Systine, PharmSelex

Member, Board of Trustees Gordon Research Conferences 1988-1994

Cofounder Molecular Simulations Inc. (now named Accelrys) (1984), San Diego CA. Member Board of Directors (84-95), Chairman Board (84-91)

Cofounder Schrödinger Inc. (1990), New York City. Member Board of Directors 1990-2000; Chairman Scientific Advisory for Materials (2012-present)

Cofounder Systine Inc. Pasadena CA (2001), Chairman Board of Directors 2003-present

Cofounder-Allozyne Inc. (2005), Seattle Washington, Member SAB (2005-present)

Cofounder-AquaNano Inc Pasadena CA (2009), Chairman SAB (2009-present)

Cofounder QioMed (Los Angeles) 2009, Member Board Directors (2009-present)

Current Government Research Funding: Department of Energy, Defense Advanced Research Projects Agency, Army Research Office, Office of Naval Research, National Science Foundation, National Institutes of Health, ARPA-E

Current Industrial Funding: Cargill Corp, Bosch Energy Research, Dow-Corning, Asahi Kasei, Panasonic

Autobiography of the early period in Goddard's career: "Critical Points and Random Events that Shaped the Early Career of William A. Goddard III" in J. Phys. Chem. A 104, 2147 (2000) (the Goddard Festschrift containing articles celebrating Goddard's 60th birthday

http://www.wag.caltech.edu/publications/sup/pdf/434.pdf

Scientific genealogy: see http://phdtree.org/scholar/goddard-william-a-iii/

- William A. Goddard III obtained his Ph.D. in Engineering Science with a minor in Physics in October 1964 from Prof. Pol Duwez, Professor of Materials Science at Caltech, Pasadena CA
- Pol Duwez received his D.Sc. in 1933 from Prof. Emile Henriot, Professor of Physics at the Free University Brussels in Belgium
- Emile Henriot received his D.Sc. in Physics in 1912 from Prof. Marie Curie at the Sorbonne University, Paris France
- Marie Sklodowska Curie received her D.Sc. in 1903 from Prof. Gabriel Lippmann at the ESPCI University of Paris, Paris France. She was awarded the Nobel prize Physics 1903 and the Nobel prize Chemistry 1911
- Gabriel Lippmann received his PhD Physics from U. Heidleberg in 1874 from Gustav Kirchhoff. He was awarded the Nobel Prize physics in 2008 for color photography
- Gustav Kirchhoff received his PhD in 1847 from Franz Ernst Neumann at the Albertus University of Kōnigsberg
- Franz Ernst Neumann received his PhD in 1825 from Christian Samuel Weiss at the Friedrich-Wilhelms University of Berlin
- Christian Samuel Weiss received his PhD from the University of Leipzig in 1809 from Abraham Gottlob Werner and Rene Just Haüy
- Abraham Gottlob Werner received his PhD in 1774 from Johann Carl Gehler at the University of Leipzig and a PhD from the Freiberg University of Mining and Technology from Karl Eugen Pabst von Ohain