WILLIAM A. GODDARD, III
California Institute of Technology:
Charles and Mary Ferkel Professor of Chemistry, Materials Science, and Applied Physics
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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).

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 (1986)
- Elected Fellow of American Physical Society (1988)
- Winner American Chemical Society Award for Computers in Chemistry (1988)
- Elected Fellow of American Association for the Advancement of Science (1990)
- Awarded Feynman Prize for Nanotechnology Theory (1999)
- Awarded Richard Chase Tolman Prize from the Southern California Section ACS (2000)
- Named ISI Highly Cited Chemist for 1981-2001 (http://isihighlycited.com)
- Awarded Honoris Causa Philosophia Doctorem, Chemistry, Uppsala U., Sweden, January 2004
- 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)
- Elected Fellow of American Academy of Arts and Sciences (2010)

- Awarded NASA Space Sciences Award for polymer films (2012)
- World Class University Professor in the Energy, Environment, Water, Sustainability (EEWS) Graduate School; Korea Advanced Institute of Science and Technology (KAIST), Daejeon, Korea (2009-2013)
- Award Distinguished Scientific Achievement Catalysis 7th World Congress Oxidation Catalysis (2013)
- IISc-DST Centenary Chair Professor at the Indian Institute of Science, Bangalore India, 2015
- Named ISI Highly Cited Chemist for 2014 (http://isihighlycited.com)
- Named ISI Highly Cited Chemist for 2015 (http://isihighlycited.com)
- Named ISI Highly Cited Chemist for 2016 (http://isihighlycited.com)

Selected Recent Research publications: total over 1305. (H index = 148; I-10 index 1098)
https://sites.google.com/view/wag-pubs
https://scholar.google.com/citations?user=yMZlErUAAAAJ&hl=en

1. **Grand canonical electronic density-functional theory: Algorithms and applications to electrochemistry;** Ravishankar Sundararaman, William A. Goddard III, and Tomas A. Arias; Citation: The Journal of Chemical Physics 146, 114104 (2017); wag1206
2. **Ultrahigh Mass Activity for Carbon Dioxide Reduction Enabled by Gold-iron Core-shell Nanoparticles.** J Sun, Kun and Cheng, Tao and Wu, Lina and Hu, Yongfeng and Zhou, Jigang and MacLennan, Aimee and Jiang, Zhaohua and Gao, Yunzhi and Goddard, William A., III and Wang, Zhijiang . Amer. Chem.Soc.; DOI: 10.1021/jacs.7b09251. (2017) wag1240
3. **Nature of the active sites for CO reduction on copper nanoparticles; suggestions for optimizing performance.** T. Cheng; H. Xiao & W.A. Goddard III. JACS 139 (34):11642–11645 (2017)
4. **Full atomistic reaction mechanism with kinetics for CO reduction on Cu(100) from ab initio molecular dynamics free-energy calculations at 298 K.** T. Cheng; H. Xiao & W.A. Goddard III. Proceedings of the National Academy of Sciences of the United States of America 114 (8):1795–1800 (2017)
5. **Explanation of Dramatic pH-Dependence of Hydrogen Binding on Noble Metal Electrode: Greatly Weakened Water Adsorption at High pH.** T. Cheng; L. Wang; B.V. Merinov & I.G. William A. Journal of the American Chemical Society (2018)

Five Other Publications

6. **Defect-enriched iron fluoride-oxide nanoporous thin films bifunctional catalyst for water splitting;** Xiujun Fan, Yuanyue Liu, Shuai Chen, Jianjian Shi, Juanjuan Wang, Ailing Fan, Wenyan Zan, Sidian Li, William A. Goddard III & Xian-Ming Zhang; Nature Communicationsvolume 9, Article number: 1809 (2018); doi:10.1038/s41467-018-04248-y
7. **In silico discovery of new dopants for Fe-doped Ni oxyhydroxides (Ni1-xFexOOH) catalysts for oxygen evolution reaction;** Hyeyoung Shin, Hai Xiao, and William A. Goddard; J. Am. Chem. Soc., DOI: 10.1021/jacs.8b02225 wag1263
8. **The synergy between Fe and Ni in the Optimal Performance of Fe,Ni)OOH Catalysts for the Oxygen Evolution Reaction**; Hai Xiao, Hyeyoung Shin, and William A. Goddard; (2018) Proceedings of the National Academy of Sciences, 2018 https://doi.org/10.1073/pnas.1722034115 wag1264
9. **Ultrafine jagged platinum nanowires enable ultrahigh mass activity for the oxygen reduction reaction;** Zhao, Cheng, Fortunelli,and Chen, Chih-Yen and Yu, Rong and Zhang, Qinghua and Gu, Lin and Merinov, Boris V. and Lin, Zhaoyang and Zhu, Enbo and Yu, Ted and Jia, Qingying and Guo, Jinghua and Zhang, Liang and Goddard, William A., III and Huang, Yu and Duan, Xiangfeng (2016) Science, 354 (6318). pp. 1414-1419.