

William H. Green

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EDUCATION:

1988 Ph.D., Physical Chemistry, University of California, Berkeley (advisor: C. Bradley Moore)
1983 B.A. with Highest Honors, Chemistry, Swarthmore College, Pennsylvania

PROFESSIONAL EXPERIENCE:

2012-2015 Executive Officer, Department of Chemical Engineering, MIT.
1997-Present Faculty, Department of Chemical Engineering, MIT.
1991-1997 Principal Investigator, Exxon Research & Engineering Corporate Research Laboratory
1991 Postdoctoral Research Associate, University of Pennsylvania (Advisor: M.I. Lester)
1989-1990 The Darwin Research Fellow, Darwin College, Cambridge Univ. (Advisor: N.C. Handy)
Summer 1983 Research Chemist, DuPont Experimental Station.

SELECTED HONORS AND AWARDS

The ACS Glenn Award in Fuel Chemistry (three times: 2013 and 2009 and 2004)
for best paper on Fuel Chemistry presented at the American Chemical Society national meeting
Hoyt C. Hottel Chair of Chemical Engineering, MIT (2009)
C.M. Mohr Outstanding Teaching Award, MIT (2006)
Elected to Executive Board, Eastern States Section, Combustion Institute (2006)
Certificate of Merit, ACS Environmental Chemistry Division (2005)
E.W. Thiele Lectureship Award, Notre Dame Univ. (2004)
NSF CAREER Award (1999)
Elected and re-elected several times to represent Precinct 7 in Belmont Town Meeting (1998-2012)
The Charles & Katherine Darwin Research Fellow, Darwin College, Cambridge University (1989-1990)
NSF Postdoctoral Fellowship in Chemistry (1989-1990)
NSF-NATO Postdoctoral Fellowship in Science & Engineering (1989)
NSF Graduate Research Fellowship (1983-1986)

CONTRIBUTIONS TO THE SCIENTIFIC COMMUNITY

Editor-in-Chief, *International Journal of Chemical Kinetics* (2008-2013)
Associate Editor, *International Journal of Chemical Kinetics* (2003-2008)
Convenor and Organizer of 7th International Conference on Chemical Kinetics (2011).
Steering Committee, 8th and 9th International Conferences on Chemical Kinetics (2013, 2015)
Organizer of more than a dozen sessions at AIChE and ACS National Meetings (1999-2013).
Executive Committee, DOE Energy Frontier Research Center on Combustion Science (2009-2015).
Education of scientific leaders: Fifteen of my former PhD students and postdocs now hold tenure-track faculty positions; several others are leaders in industrial research.

RESEARCH

Leader of 20-member research group focusing on chemical kinetics important for energy and environmental problems. World leader in computer-aided kinetic modeling based on first-principles calculations, including solvent and pressure effects; also performs experiments to test the models, and invents numerical methods relevant to chemical kinetic and reacting flow simulations. Author of 2 US Patents, on novel CO₂ Capture Sorbents and a Small-Scale Gas-to-Liquids Process. Author of more than 200 journal articles, cited more than 7,000 times (h-index=51).

TEN SELECTED PUBLICATIONS:

- 1) A. Jalan, I.M. Alecu, R. Meana-Paneda, J. Aguilera-Iparraguirre, K.R. Yang, S.S. Merchant, D.G. Truhlar, and W.H. Green, "New pathways for formation of acids and carbonyl products in low-temperature oxidation: The Korcek decomposition of γ -keto hydroperoxides." *Journal of the American Chemical Society* **135**, 11100-11114 (2013).
- 2) Nils Hansen, Shamel S. Merchant, Michael R. Harper, and William H. Green, "The Predictive Capability of an Automatically Generated Combustion Chemistry Mechanism: Chemical Structures of Premixed *iso*-Butanol Flames," *Combustion & Flame* **160**, 2343-2351 (2013).
- 3) Joshua W. Allen, C. Franklin Goldsmith, and William H. Green, "Automatic Estimation of Pressure-Dependent Rate Coefficients", *Physical Chemistry Chemical Physics* **14**(3), 1131 (2012).
- 4) William H. Green, "Predictive Kinetics: A New Approach for the 21st Century", *Advances in Chemical Engineering* **32**, 1-50 (2007).
- 5) Binita Bhattacharjee, Douglas A. Schwer, Paul I. Barton, & William H. Green, Jr., "Optimally-Reduced Kinetic Models: Reaction Elimination in Large-Scale Kinetic Mechanisms", *Combustion & Flame* **135**, 191-208 (2003).
- 6) Raman Sumathi and William H. Green, "A priori Rate Constants for Kinetic Modeling", *Theoretical Chemistry Accounts* **108**, 187-213 (2002).
- 7) David V. Avila, Keith U. Ingold, Janusz Luszyk, William H. Green, and Daniel R. Procopio, "Dramatic Solvent Effects on the Absolute Rate Constants for Abstraction of the Hydroxylic Hydrogen Atom from *tert*-Butyl Hydroperoxide and Phenol by the Cumyloxy Radical. The Role of Hydrogen Bonding.", *Journal of the American Chemical Society* **117**, 2929-30 (1995).
- 8) William H. Green, C. Bradley Moore, and William F. Polik, "Unimolecular Reaction Rates and Transition States", *Annual Review of Physical Chemistry* **43**, 591-626 (1992).
- 9) William H. Green and Marsha I. Lester, "A Perturbation Theory Guide to Open-Shell Complexes: OH-Ar ($X^2\Pi$)", *Journal of Chemical Physics* **96**, 2573 (1992).
- 10) William H. Green, Nicholas C. Handy, Peter J. Knowles, and Stuart Carter, "Theoretical Assignment of the Visible Spectrum of Singlet Methylene", *Journal of Chemical Physics* **94**, 118 (1991).