Publications of William A. Goddard III

A. Biological Systems

A.1. Proteins

306-Protein Simulations using Techniques Suitable for Very Large Systems: the Cell Multipole Method for Nonbond Interactions and the Newton−Euler Inverse Mass Operator Method for Internal Coordinate Dynamics. A. M. Mathiowetz, A. Jain, N. Karasawa, and W. A. Goddard III. *Proteins* **20**, 227 (1994).

336-Prediction of Polyelectrolyte Polypeptide Structures using Monte Carlo Conformational Search Methods with Implicit Solvation Modeling. J. S. Evans. S. I. Chan, and W. A. Goddard III. *Protein Sci*. **4**, 2019 (1995).

361-The Pentamer Channel Stiffening Model for Drug Action on Human Rhinovirus HRV-1A. N. Vaidehi and W. A. Goddard III. *Proc. Natl. Acad. Sci. U.S.A.* **94**, 2466 (1997).

387-Kinetic Steps for Alpha Helix Formation. R. A. Bertsch, N. Vaidehi, S. I. Chan, and W. A. Goddard III. *Protein Sci*. **33**, 1 (1998).

378-The Role of Enzyme Distortion in the Single-Displacement Mechanism of Family 19 Chitinases. K. A. Brameld and W. A. Goddard III, Proc. Natl. Acad. Sci. **95**, 4278 (1998).

380-Substrate Distortion to a Boat Conformation at Subsite -1 is Critical in the Mechanism of Family 18 Chitinases, K. A. Brameld and W. A. Goddard III. *J. Am. Chem. Soc*. **120**, 3571 (1998).

382-Substrate Assistance in the Mechanism of Family 18 Chitinases: Theoretical Studies of Potential Intermediates and Inhibitors, K. A. Brameld, W. D. Shrader, B. Imperiali, and W. A. Goddard III. *J. Mol. Biol.* **280**, 913 (1998).

392-Effects of Pressure on the Structure of Metmyoglobin: Molecular Dynamics Predictions for Pressure Unfolding Through a Molten Globule Intermediate. W. B. Floriano, M. A. Nascimento, G. B. Domont, and W. A. Goddard III. *Protein Sci*. **7**, 2301 (1998).

410-Atomic Level Simulation Models for Biological Systems. N. Vaidehi and W. A. Goddard III, In *Computational Models of Molecular and Cellular Interactions*, Chapter 7, J. Bower and H. Bolouri, Editors (1999).

A.2. Nucleic Acids

253-Predictions of Structural Elements for the Binding of Hin Recombinase with the Hix Site of DNA. K. W. Plaxco, A. M. Mathiowetz, and W. A. Goddard III. *Proc. Natl. Acad. Sci. U.S.A.* **86**, 9841 (1989).

276-Protein Stitchery: Design of a Protein for Selective Binding to a Specific DNA Sequence. C. Park, W. A. Goddard, III, and J. L. Campbell. *Proc. Natl. Acad. Sci. U.S.A.* **89**, 9094 (1992).

291-Design Superiority of Palindromic DNA Sites for Site-Specific Recognition of Proteins: Tests Using Protein Stitchery. C. M. Park, J. L. Campbell, and W. A. Goddard III. *Proc. Natl. Acad. Sci. U.S.A.* **90**, 4892 (1993).

322-Design and Synthesis of a New Peptide Recognizing a Specific 16-Base-Pair Site of DNA. C. Park, J. L. Campbell, and W. A. Goddard III. *J. Am. Chem. Soc.* **117**, 6287 (1995).

342-Can the Monomer of the Leucine Zipper Proteins Recognize the Dimer Binding Site without Dimerization? C. Park, J. L. Campbell, and W. A. Goddard III. *J. Am. Chem. Soc.* **118**, 4235 (1996).

303-Contributions of the Thymine Methyl Group to the Specific Recognition of Poly- and Mononucleotides: An Analysis of the Relative Free Energy of Solvation of Thymine and Uracil. K. W. Plaxco and W. A. Goddard III. *Biochemistry* **33**, 3050 (1994).

397-Ab Initio Quantum Mechanical Study of the Structures and Energies for the Pseudorotation of 5′-Dehydroxy Analogues of 2′-Deoxyribose and Ribose Sugars. K. A. Brameld and W. A. Goddard III. *J. Am. Chem. Soc*. **121**, 985 (1999).

A.3. Electronic States in Bioinorganics

73-Ozone Model for Bonding of an O_2 to Heme in Oxyhemoglobin. W. A. Goddard III and B. D. Olafson. *Proc. Natl. Acad. Sci. U.S.A.* **72**, 2335 (1975).

97-Molecular Description of Dioxygen Bonding in Hemoglobin. B. D. Olafson and W. A. Goddard III. *Proc. Natl. Acad. Sci. U.S.A.* **74**, 1315 (1977).

132-Theoretical Studies of the Bonding of O_2 to Hemoglobin: Implications for Cooperativity. W. A. Goddard III and B. D. Olafson. In *Biochemical and Clinical Aspects of Oxygen*; W. S. Caughey, Ed. (Academic Press, Inc., New York, 1979); pp 87−123.

147-Theoretical Studies of Oxygen Binding. W. A. Goddard III and B. D. Olafson. *Ann. N.Y. Acad. Sci*. **367**, 419 (1981).

161-The Electronic Spectra of Hb, HbO_2, and HbCO. B. D. Olafson and W. A. Goddard III. In *Hemoglobin and Oxygen Binding*; Chien Ho, Ed. (Elsevier North-Holland, New York, 1982); pp 83−89.

99-Theoretical Studies of the Oxidized and Reduced States of a Model for the Active Site of Rubredoxin. R. A. Bair and W. A. Goddard III. *J. Am. Chem. Soc*. **99**, 3505 (1977).

119-Theoretical Studies of the Ground and Excited States of a Model of the Active Site in Oxidized and Reduced Rubredoxin. R. A. Bair and W. A. Goddard III. *J. Am. Chem. Soc*. **100**, 5669 (1978).

133-Singlet Molecular Oxygen Chemistry and Implications for Flavin-Cofactor Hydroxylations. W. A. Goddard III and L. B. Harding. In *Biochemical and Clinical Aspects of Oxygen*; W. A. Caughey, Ed. (Academic Press, Inc., New York, 1979); pp 513−555.

308-Electronic Structures of Halogenated Porphyrins: Spectroscopic Properties of $ZnTFPPX_8$ ($TFPPX_8$ = Octa-β-halotetrakis(pentafluorophenyl)porphyrin; X = Cl, Br). T. Takeuchi, H. B. Gray, and W. A. Goddard III. *J. Am. Chem. Soc*. **116**, 9730 (1994).

337-Ruffling in a Series of Nickel(II) *meso*-Tetrasubstituted Porphyrins as a Model for the Conserved Ruffling of the Heme of Cytochromes *c*. W. Jentzen, M. C. Simpson, J. D. Hobbs, X. Song, T. Ema, N. Y. Nelson, C. J. Medforth, K. M. Smith, M. Veyrat, M. Mazzanti, R. Ramasseul, J.-C. Marchon, T. Takeuchi, W. A. Goddard III, and J. A. Shelnutt. *J. Am. Chem. Soc.* **117**, 11085 (1995).

395-Chromophore-in-Protein Modeling of the Structures and Resonance Raman Spectra for Type 1 Copper Proteins. D. Qiu, S. Dasgupta, P. M. Kozlowski, W. A. Goddard III, and T. G. Spiro. *J. Am. Chem. Soc*. **120**, 12791 (1998).

A.4. Protein Folding

400-The Topomer-Sampling Model of Protein Folding. D. A. Debe, M. J. Carlson, and W. A. Goddard III. *Proc. Natl. Acad. Sci. U.S.A.* **96**, 2596 (1999).

10.1021/jp000183b CCC: $19.00
Published on Web 02/23/2000

405-Protein Fold Determination from Sparse Distance Restraints; The Restrained Generic Protein Direct Monte Carlo Method. D. A. Debe, M. J. Carlson, J. Sadanobu, S. I. Chan, and W. A. Goddard III. *J. Phys. Chem. B* **103**, 3001 (1999).

422-First Principles Prediction of Protein Folding Rates. D. A. Debe and W. A. Goddard III. *J. Mol. Biol*. **294**, 619 (1999).

A.5. Drug Design

407-Mechanism and Energetics for Complexation of ^{90}Y with 1,4,7,10-Tetraazacyclododecane-1,4,7,10-Tetraacetic Acid (DOTA), a Model for Cancer Radioimmunotherapy. Y. H. Jang, M. Blanco, S. Dasgupta, D. A. Keire, J. E. Shively, and W. A. Goddard III. *J. Am. Chem. Soc*. **121**, 6142 (1999).

B. Reactions and Catalysis

B.1. Selection Rules for Chemical Reactions

28-The Orbital Phase Continuity Principle and Selection Rules for Concerted Reactions. W. A. Goddard III. *J. Am. Chem. Soc*. **92**, 7520 (1970).

34-Selection Rules for Chemical Reactions Using the Orbital Phase Continuity Principle. W. A. Goddard III. *J. Am. Chem. Soc*. **94**, 793 (1972).

182-2_s+2_s Reactions at Transition Metals: I. The Reactions of D_2 with Cl_2TiH^+, Cl_2TiH, and Cl_2ScH. M. L. Steigerwald and W. A. Goddard III. *J. Am. Chem. Soc*. **106**, 308 (1984).

B.2. Organic Reaction Intermediates

33-Theoretical Investigations of the Trimethylene Biradical. P. J. Hay, W. J. Hunt, and W. A. Goddard III. *J. Am. Chem. Soc*. **94**, 638 (1972).

81-The Ground and Excited States of Trimethylenemethane. J. H. Davis and W. A. Goddard III. *J. Am. Chem. Soc*. **98**, 303 (1976).

102-Electronic States of Trimethylenemethane. J. H. Davis and W. A. Goddard III. *J. Am. Chem. Soc*. **99**, 4242 (1977).

84-Vinylmethylene and the Ring Opening of Cyclopropene: Ab Initio Generalized Valence Bond and Configuration Interaction Studies. J. H. Davis, W. A. Goddard III, and R. G. Bergman. *J. Am. Chem. Soc*. **98**, 4015 (1976).

95-Vinylmethylene: Theoretical Investigations. J. H. Davis, W. A. Goddard III, and R. G. Bergman. *J. Am. Chem. Soc*. **99**, 2427 (1977).

B.3. Organic Reaction Mechanisms

71-The Electronic Structure of the Criegee Intermediate: Ramifications for the Mechanism of Ozonolysis. W. R. Wadt and W. A. Goddard III. *J. Am. Chem. Soc*. **97**, 3004 (1975).

122-Mechanisms of Gas Phase and Liquid Phase Ozonolysis. L. B. Harding and W. A. Goddard III. *J. Am. Chem. Soc*. **100**, 7180 (1978).

103-Intermediates in the Chemiluminescent Reaction of Singlet Oxygen with Ethylene: Ab Initio Studies. L. B. Harding and W. A. Goddard III. *J. Am. Chem. Soc*. **99**, 4520 (1977).

114-Mechanistic Implications of the Stereochemistry of Singlet Oxygen-Olefin Reactions. L. B. Harding and W. A. Goddard III,. *Tetrahedron Lett*. **747**, (1978).

134-The Mechanism of the Ene Reaction of Singlet Oxygen with Olefins. L. B. Harding and W. A. Goddard III. *J. Am. Chem. Soc*. **102**, 439 (1980).

128-Theoretical Studies of the Oxy Anionic Substituent Effect. M. L. Steigerwald, W. A. Goddard III, and D. A. Evans. *J. Am. Chem. Soc*. **101**, 1994 (1979).

168-Energetics and Mechanisms for Reactions Involving Nitrosamide, Hydroxy Diazenes, and Diimide N-Oxides. C. J. Casewit and W. A. Goddard III. *J. Am. Chem. Soc*. **104**, 3280 (1982).

357-Mechanism of Atmospheric Photooxidation of Aromatics—A Theoretical Study. J. M. Andino, J. N. Smith, R. C. Flagan, W. A. Goddard III, and J. H. Seinfeld. *J. Phys. Chem*. **100**, 10967 (1996).

B.4. Chemisorbed Species on Metal Surfaces

110-Theoretical Studies of the Geometries of O and S Overlayers on the (100) Surface of Nickel. S. P. Walch and W. A. Goddard III. *Solid State Commun*. **23**, 907 (1977).

115-Theoretical Studies of the Bonding of Sulfur to Models of the (100) Surface of Nickel. S. P. Walch and W. A. Goddard III. *Surf. Sci*. **72**, 645 (1978).

116-Theoretical Studies of the Bonding of Oxygen to Models of the (100) Surface of Nickel. S. P. Walch and W. A. Goddard III. *Surf. Sci*. **75**, 609 (1978).

153-Evidence for Two States of Chemisorbed Oxygen on Ni(100). T. H. Upton and W. A. Goddard III. *Phys. Rev. Lett*. **46**, 1635 (1981).

123-Electronic Properties of Metal Clusters (Ni_{13} to Ni_{87}) and Implications for Chemisorption. C. F. Melius, T. H. Upton, and W. A. Goddard III. *Solid State Commun*. **28**, 501 (1978).

127-Chemisorption of Atomic Hydrogen on Large Nickel Cluster Surfaces. T. H. Upton and W. A. Goddard III. *Phys. Rev. Lett*. **42**, 472 (1979).

129-Theoretical Studies of Nickel Clusters and Chemisorption of Hydrogen. T. H. Upton, W. A. Goddard III, and C. F. Melius. *J. Vac. Sci. Technol*. **16**, 531 (1979).

135-Theoretical Studies of the Dissociative Absorption of H_2 on Ni(001) Using Ab Initio Parameterized LEPS Calculations. V. I. Avdeev, T. H. Upton, W. H. Weinberg, and W. A. Goddard III. *Surf. Sci*. **95**, 391 (1980).

146-Chemisorption of H, Cl, Na, O, and S Atoms on Ni(100) Surfaces: A Theoretical Study Using Ni_{20} Clusters. T. H. Upton and W. A. Goddard III. *Crit. Rev. Solid State Mater. Sci*. **10**, 261 (1981).

160-Geometry, Vibrational Frequencies, and Ionization Potentials for CO/Ni(100); Explanation of the Disappearance of the 5s Peak in PES. J. N. Allison and W. A. Goddard III. *Surf. Sci*. **110**, L615 (1981).

166-Theoretical Studies of CO/Ni(100): Geometry, Vibrational Frequencies, and Ionization Potentials for the On-Top Site. J. N. Allison and W. A. Goddard III. *Surf. Sci*. **115**, 553 (1982).

175-Theoretical Vibrational Frequencies for NH_x and CH_x Reactive Intermediates on Ni(100) and Ni(111) Surfaces. J. J. Low and W. A. Goddard III. *J. Electron Spectrosc*. **30**, 27 (1983).

393-Chemisorption of Organics on Platinum: Part I. The Interstitial Electron Model. J. Kua and W. A. Goddard III. *J. Phys. Chem*. **102**, 9481 (1998).

394-Chemisorption of Organics on Platinum: Part II. Chemisorption of C_2H_x and CH_x on Pt(111). J. Kua and W. A. Goddard III. *J. Phys. Chem*. **102**, 9492 (1998).

421-Oxidation of Methanol on Second and Third Row Group VIII Transition Metals (Pt, Ir, Os, Pd, Rh, and Ru): Application to Direct Methanol Fuel Cells. J. Kua and W. A. Goddard III. *J. Am. Chem. Soc*. **121**, 10928 (1999).

B.5. Reaction Rates at Surfaces

174-Classical Stochastic Diffusion Theory for Desorption of Atoms and Molecules from Solid Surfaces. A. Redondo, Y. Zeiri, and W. A. Goddard III. *Phys. Rev. Lett*. **49**, 1847 (1982).

176-Rates of Molecular Desorption from Solid Surfaces: Adsorption Site Dependence for CO on Ni(100). J. N. Allison, Y. Zeiri, A. Redondo, and W. A. Goddard III. *Chem. Phys. Lett*. **97**, 387 (1983).

177-Classical Stochastic Diffusion Theory for Desorption from Solid Surfaces. Y. Zeiri, A. Redondo, and W. A. Goddard III. *Surf. Sci.* **131**, 221 (1983).

180-Application of Transition State Theory to Desorption from Solid Surfaces: Ammonia on Ni(111). A. Redondo, Y. Zeiri, J. J. Low, and W. A. Goddard III. *J. Chem. Phys*. **79**, 6410 (1983).

181-Rates of Desorption from Solid Surfaces: Coverage Dependence. A. Redondo, Y. Zeiri, and W. A. Goddard III. *Surf. Sci.* **136**, 41 (1984).

185-Classical Stochastic Diffusion Theory for Thermal Desorption from Solid Surfaces. A. Redondo, Y. Zeiri, and W. A. Goddard III. *J. Vac. Sci. Technol. B* **2**, 550 (1984).

186-Desorption Rates at Electrode/Electrolyte Interfaces. Y. Zeiri, A. Redondo, and W. A. Goddard III. *J. Electrochem. Soc*. **131**, 1639 (1984).

205-A Theoretical Study of Collision-Induced Desorption Spectroscopy from Si(111) Surfaces. Y. Zeiri, J. J. Low, and W. A. Goddard III. *J. Chem. Phys*. **84**, 2408 (1986).

220-Dissociation Energetics of SiF Systems of Relevance to Etching Reactions. B. J. Garrison and W. A. Goddard III. *J. Chem. Phys*. **87**, 1307 (1987).

227-A Reaction Mechanism for Fluorine Etching of Silicon. B. J. Garrison and W. A. Goddard III. *Phys. Rev. B* **36**, 9805 (1987).

B.6. Transition Metal Molecules

56-The Generalized Valence Bond Description of Titanium Carbonyl. A. P. Mortola and W. A. Goddard III. *J. Am. Chem. Soc.* **96**, 1 (1974).

90-Generalized Valence Bond Description of the Low-Lying States of NiCO. S. P. Walch and W. A. Goddard III. *J. Am. Chem. Soc.* **98**, 7908 (1976).

100-Generalized Valence Bond Studies of the Electronic States of $NiCH_2$ and $NiCH_3$. A. K. Rappé, and W. A. Goddard III. *J. Am. Chem. Soc.* **99**, 3966 (1977).

111-Interaction of Acetylene and Ethylene with Nickel Atom. T. H. Upton and W. A. Goddard III. *J. Am. Chem. Soc.* **100**, 321 (1978).

117-Experimental and Theoretical Studies of $Ni_n(C_2H_4)_m$: Synthesis, Vibrational and Electronic Spectra, and Generalized Valence Bond-Configuration Interaction Studies; The Metal Atom Chemistry and a Localized Bonding Model for Ethylene Chemisorbed on Bulk Nickel. G. A. Ozin, W. J. Power, T. H. Upton, and W. A. Goddard III. *J. Am. Chem. Soc.* **100**, 4750 (1978).

112-Electronic States of the NiO Molecule. S. P. Walch and W. A. Goddard III. *J. Am. Chem. Soc.* **100**, 1338 (1978).

118-The Electronic States of Ni_2 and Ni_2^+. T. H. Upton and W. A. Goddard III. *J. Am. Chem. Soc.* **100**, 5659 (1978).

148-Theoretical Studies of Reactions at Transition Metal Centers. A. K. Rappé, and W. A. Goddard III. In *Potential Energy Surfaces and Dynamics Calculations*; D. G. Truhlar, Ed. (Plenum Press, New York, 1981); pp 661−684.

149-The "Sextuple" Bond of Cr_2. M. M. Goodgame and W. A. Goddard III. *J. Phys. Chem*. **85**, 215 (1981).

164-Nature of the Mo−Mo and Cr−Cr Multiple Bonds: A Challenge for the Local Density Approximation. M. M. Goodgame and W. A. Goddard III. *Phys. Rev. Lett*. **48**, 135 (1982).

192-Modified Generalized Valence Bond Method: A Simple Correction for the Electron Correlation Missing in Generalized Valence Bond Wavefunctions; Prediction of Double Well States for Cr_2 and Mo_2. M. M. Goodgame and W. A. Goddard III. *Phys. Rev. Lett*. **54**, 661 (1985).

152-Flexible d Basis Sets for Sc Through Cu. A. K. Rappé, T. A. Smedley, and W. A. Goddard III. *J. Phys. Chem*. **85**, 2607 (1981).

162-Titanacyclobutane: Structural Considerations. A. K. Rappé and W. A. Goddard III. *J. Am. Chem. Soc.* **104**, 297 (1982).

199-Dichlorotitanacyclopropane. The Structure and Reactivity of a Metallacyclopropane. M. L. Steigerwald and W. A. Goddard III. *J. Am. Chem. Soc.* **107**, 5027 (1985).

228-Metallacyclobutadiene Versus Metallatetrahedrane Structures for $Cl_3MoC_3H_3$ Complexes. E. V. Anslyn, M. J. Brusich, and W. A. Goddard III. *Organometallics* **7**, 98 (1988).

179-The Lower Electronic States of MoN. J. N. Allison and W. A. Goddard III. *Chem. Phys*. **81**, 263 (1983).

238-Early Versus Late Transition Metal−Oxo Bonds: The Electronic Structure of VO^+ and RuO^+. E. A. Carter and W. A. Goddard III. *J. Phys. Chem*. **92**, 2109 (1988).

184-The Chromium Methylidene Cation: $CrCH_2^+$. E. A. Carter and W. A. Goddard III. *J. Phys. Chem*. **88**, 1485 (1984).

210-Electronic States of Chromium Carbene Ions Characterized by High Resolution Translational Energy Spectroscopy. M. A. Hanratty, E. A. Carter, J. L. Beauchamp, W. A. Goddard III, A. J. Illies, and M. T. Bowers. *Chem. Phys. Lett*. **128**, 239 (1986).

211-Bonding in Transition-Metal Methylene Complexes: 2. $(RuCH_2)^+$, A Complex Exhibiting Low-Lying Triplet Methylidene-Like and Singlet Carbene-Like States. E. A. Carter and W. A. Goddard III. *J. Am. Chem. Soc.* **108**, 2180 (1986).

213-Bonding in Transition-Metal Methylene Complexes: 3. Comparison of Cr and Ru Carbenes; Predictions of Stable $L_nM(CXY)$ Systems. E. A. Carter and W. A. Goddard III. *J. Am. Chem. Soc.* **108**, 4746 (1986).

251-Structures and Reactivity of Neutral and Cationic Molybdenum Methylidene Complexes. E. V. Anslyn and W. A. Goddard III. *Organometallics* **8**, 1550 (1989).

311-Energetics of Third-Row Transition Metal Methylidene Ions MCH^+_2 (M = La, Hf, Ta, W, Re, Os, Ir, Pt, Au). K. K. Irikura and W. A. Goddard III. *J. Am. Chem. Soc.* **116**, 8733 (1994).

203-Electron Correlation Effects in Ligand Field Parameters and Other Properties of CuF_2. S. Yu. Shashkin and W. A. Goddard III. *J. Phys. Chem*. **90**, 255 (1986).

225-The Bond Energy and Other Properties of the Re−Re Quadruple Bond. D. C. Smith and W. A. Goddard III. *J. Am. Chem. Soc.* **109**, 5580 (1987).

234-Theoretical Studies of Silicon-Containing Molecules. D. S. Horowitz and W. A. Goddard III. *J. Mol. Struct.: THEOCHEM* **163**, 207 (1988).

229-Thermochemistry of Silaethylene and Methylsilylene from Experiment and Theory. S. K. Shin, K. K. Irikura, J. L. Beauchamp, and W. A. Goddard III. *J. Am. Chem. Soc.* **110**, 24 (1988).

258-Singlet−Triplet Energy Gaps in Chlorine-Substituted Methylenes and Silylenes. S. K. Shin, W. A. Goddard III, and J. L. Beauchamp. *J. Phys. Chem*. **94**, 6963 (1990).

262-Singlet−Triplet Energy Gaps in Fluorine-Substituted Methylenes and Silylenes. S. K. Shin, W. A. Goddard III, and J. L. Beauchamp. *J. Chem. Phys*. **93**, 4986 (1990).

277-Inequivalence of Equivalent Bonds; Symmetry Breaking in $Co(CH_3)^{2+}$. J. K. Perry, W. A. Goddard III, and G. Ohanessian. *J. Chem. Phys.* **97**, 7560 (1992).

292-Molecular Complexes of Small Alkanes with Co^+. J. K. Perry, G. Ohanessian, and W. A. Goddard III. *J. Phys. Chem.* **97**, 5238 (1993).

319-Experimental and Theoretical Studies of $Co(CH_4)_x^+$ with $x = 1-4$. C. L. Haynes, P. B. Armentrout, J. K. Perry, and W. A. Goddard III. *J. Phys. Chem*. **99**, 6340 (1995).

305-Trends on Sc*−Alkyl Bond Strengths. J. K. Perry and W. A. Goddard III. *J. Am. Chem. Soc.* **116**, 5013 (1994).

B.7. Reaction Mechanisms for Inorganic and Organometallic Catalysts

92-Methanation of CO over Ni Catalyst: A Theoretical Study. W. A. Goddard III, S. P. Walch, A. K. Rappé, T. H. Upton, and C. F. Melius. *J. Vac. Sci. Technol*. **14**, 416 (1977).

217-Methylidene Migratory Insertion into an Ru−H Bond. E. A. Carter and W. A. Goddard III. *J. Am. Chem. Soc.* **109**, 579 (1987).

236-Modeling Fischer−Tropsch Chemistry: The Thermochemistry and Insertion Kinetics of $ClRuH(CH_2)$. E. A. Carter and W. A. Goddard III. *Organometallics* **7**, 675 (1988).

139-Bivalent Spectator Oxo Bonds in Metathesis and Epoxidation of Alkenes. A. K. Rappé and W. A. Goddard III. *Nature* **285**, 311 (1980).

138-Mechanism of Metathesis and Epoxidation in Chromium and Molybdenum Complexes Containing Metal−Oxo Bonds. A. K. Rappé and W. A. Goddard III. *J. Am. Chem. Soc.* **102**, 5114 (1980).

169-Hydrocarbon Oxidation by High-Valent Group VI Oxides. A. K. Rappé and W. A. Goddard III. *J. Am. Chem. Soc.* **104**, 3287 (1982).

163-Olefin Metathesis. A Mechanistic Study of High-Valent Group VI Catalysts. A. K. Rappé and W. A. Goddard III. *J. Am. Chem. Soc.* **104**, 448 (1982).

190-Theoretical Studies of Oxidative Addition and Reductive Elimination: $H_2 + Pt(PH_3)_2 \rightarrow Pt(H)_2(PH_3)_2$. J. J. Low and W. A. Goddard III. *J. Am. Chem. Soc.* **106**, 6928 (1984).

191-Reductive Coupling of H−H, H−C, and C−C Bonds from Pd Complexes. J. J. Low and W. A. Goddard III. *J. Am. Chem. Soc.* **106**, 8321 (1984).

206-Theoretical Studies of Oxidative Addition and Reductive Elimination. 2. Reductive Coupling of H−H, H−C, and C−C Bonds from Pd and Pt Complexes. J. J. Low and W. A. Goddard III. *Organometallics* **5**, 609 (1986).

207-Geometrical Characteristics from Experiment and Theory of Isostructural Complexes Involving Pd− and Pt−Methyl Bonds. J. M. Wisner, T. J. Bartczak, J. A. Ibers, J. J. Low, and W. A. Goddard III. *J. Am. Chem. Soc.* **108**, 347 (1986).

214-Theoretical Studies of Oxidative Addition and Reductive Elimination. 3. C−H and C−C Reductive Coupling from Palladium and Platinum Bis(phosphine) Complexes. J. J. Low and W. A. Goddard III. *J. Am. Chem. Soc.* **108**, 6115 (1986).

195-Oxidative Dehydrogenation of Methanol to Formaldehyde. J. N. Allison and W. A. Goddard III. *J. Catal*. **92**, 127 (1985).

196-Active Sites on Molybdate Surfaces, Mechanistic Considerations for Selective Oxidation and Ammoxidation of Propene. J. N. Allison and W. A. Goddard III. *ACS Symposium Series No. 279, Solid State Chemistry in Catalysis*; R. K. Grasselli and J. F. Brazdil, Eds. (American Chemical Society, Washington, DC, 1985); pp 23−36.

241-The Surface Atomic Oxyradical Mechanism for Ag-Catalyzed Olefin Epoxidation. E. A. Carter and W. A. Goddard III. *J. Catal.* **112**, 80 (1988).

245-Chemisorption of Oxygen, Chlorine, Hydrogen, Hydroxide, and Ethylene on Silver Clusters: A Model for the Olefin Epoxidation Reaction. E. A. Carter and W. A. Goddard III. *Surf. Sci.* **209**, 243 (1989).

299-Theoretical Studies of Ziegler−Natta Catalysis: Structural Variations and Tacticity Control. E. Bierwagen, J. E. Bercaw, and W. A. Goddard III. *J. Am. Chem. Soc.* **116**, 1481 (1994).

304-Mechanism and Energetics for Dehydrogenation of Methane by Gaseous Iridium Ions. J. K. Perry, G. Ohanessian, and W. A. Goddard III. *Organometallics* **13**, 1870 (1994).

375-Fluorination of Diamond−C_4F_9I and CF_3I Photochemistry on Diamond (100). V. S. Smentkowski, J. T. Yates Jr., X. Chen, and W. A. Goddard III. *Surf. Sci.* **370**, 209 (1997).

402-Sigma-Bond Metathesis Reactions of $Sc(OCD_3)^+_2$ with Water, Ethanol, and 1-Propanol: Measurements of Equilibrium Constants, Relative Bond Strengths, and Absolute Bond Strengths. K. C. Crellin, J. L. Beauchamp, W. A. Goddard III, S. Geribaldi, and M. Decouzon. *Int. J. Mass Spectrom. Ion Processes* **182/183**, 121 (1999).

C. Polymers

C.1. Dendritic Polymers

246-Starburst Dendrimers 5: Molecular Shape Control. A. M. Naylor, W. A. Goddard III, G. E. Kiefer, and D. A. Tomalia. *J. Am. Chem. Soc.* **111**, 2339 (1989).

248-Application of Simulation and Theory to Biocatalysis and Biomimetics. A. M. Naylor and W. A. Goddard III. In *Biocatalysis and Biomimetics ACS Symposium Series 392*; J. D. Burrington and D. S. Clark, Eds. (ACS, Washington, DC, 1989); Chapter 6, pp 65−87.

255-Starburst Dendrimers: Molecular Level Control of Size, Shape, Surface Chemistry, Topology, and Flexibility from Atoms to Macroscopic Matter. D. A. Tomalia, A. M. Naylor, and W. A. Goddard III. *Angew. Chem., Int. Ed. Engl.* **29**, 138−175 (1990).

370-Dynamics of Bengal Rose Encapsulated in the Meijer Dendrimer Box. P. Miklis, T. Cagin, and W. A. Goddard III. *J. Am. Chem. Soc.* **119**, 7458 (1997).

398-Poly(amidoamine) Dendrimers: A New Class of High Capacity Chelating Agents for Cu(II) Ions. M. S. Diallo, L. Balogh, A. Shafagati, J. H. Johnson Jr., W. A. Goddard III, and D. A. Tomalia. *Environ. Sci. Technol*. **33**, 820 (1999).

413-Recent Advances in Simulation of Dendritic Polymers. T. Cagin, P. J. Miklis, G. Wang, G. Zamanakos, R. Martin, H. Li, D. T. Mainz, N. Vaidehi, and W. A. Goddard III. *Mater. Res. Soc. Symp. Proc*. **543**, 299 (1999).

C.2. Bulk Polymers

263-Mechanical Properties and Force Field Parameters for Polyethylene Crystal. N. Karasawa, S. Dasgupta, and W. A. Goddard III. *J. Phys. Chem*. **95**, 2260 (1991).

280-Thermodynamic and Elastic Properties of Polyethylene at Elevated Temperatures. T. Cagin, N. Karasawa, S. Dasgupta, and W. A. Goddard III. *Mater. Res. Soc. Symp. Proc*. **278**, 61 (1992).

278-Force Fields, Structures, and Properties of Poly(vinylidene fluoride) Crystals. N. Karasawa and W. A. Goddard III. *Macromolecules* **25**, 7268 (1992).

334-Dielectric Properties of Poly(vinylidene fluoride) from Molecular Dynamics Simulations. N. Karasawa and W. A. Goddard III. *Macromolecules* **28**, 6765 (1995).

295-Polyoxymethylene: The Hessian Biased Force Field for Molecular Dynamics Simulations. S. Dasgupta, K. A. Smith, and W. A. Goddard III. *J. Phys. Chem*. **97**, 10891 (1993).

335-Hessian Biased Force Field for Polysilane Polymers. C. B. Musgrave, S. Dasgupta, and W. A. Goddard III. *J. Phys. Chem*. **99**, 13321 (1995).

353-Crystal Structures and Properties of Nylon Polymers from Theory. S. Dasgupta, W. B. Hammond, and W. A. Goddard III. *J. Am. Chem. Soc.* **118**, 12291 (1996).

C.3. Nonlinear Optical Properties

300-The Valence Bond Charge Transfer Exciton Model for Predicting Nonlinear Optical Properties (Hyperpolarizabilities and Saturation Length) of Polymeric Materials. D. Lu, G. Chen, and W. A. Goddard III. *J. Chem. Phys*. **101**, 4920 (1994).

301-The Valence Bond Charge Transfer Solvation Model for the Nonlinear Optical Properties of Charge Transfer Organic Molecules in Polar Solvents. G. Chen, D. Lu, and W. A. Goddard III. *J. Chem. Phys*. **101**, 5860 (1994).

307-Hyperpolarizabilities of Push−Pull Polyenes−Molecular Orbital and Valence Bond Charge Transfer Models. J. W. Perry, S. R. Marder, F. Meyers, D. Lu, G. Chen, W. A. Goddard III, J.-L. Brédas, and B. M. Pierce. *ACS Symposium on Polymers for Second-Order Nonlinear Optics*; G. A. Lindsay and K. D. Singer, Eds. (American Chemical Society, Washington DC, 1995); Chapter 3, p 45 .

313-Valence-Bond Charge-Transfer Model for Nonlinear Optical Properties of Charge-Transfer Organic Molecules. D. Lu, G. Chen, J. W. Perry, and W. A. Goddard III. *J. Am. Chem. Soc.* **116**, 10679 (1994).

320-Valence Bond Charge Transfer Theory for Predicting Nonlinear Optical Properties of Organic Materials. W. A. Goddard III, D. Lu, G. Chen, and J. W. Perry. *ACS Symposium Series on Computer-Aided Molecular Design; Applications in Agrochemicals, Materials, and Pharmaceuticals*; C. H. Reynolds, M. K. Holloway, and H. K. Cox, Eds. (American Chemical Society, Washington DC, 1995); Chapter 25, p 341.

333-Ab Initio Predictions of Large Hyperpolarizability Push−Pull Polymers. Julolidinyl-*n*-isoxazolone and Julolidinyl-*n*-N,N′-diethylthiobarbituric Acid. D. Lu, B. Marten, Y. Cao, M. N. Ringnalda, R. A. Friesner, and W. A. Goddard III. *Chem. Phys. Lett*. **242**, 543 (1995).

346-Saturation of the Second Hyperpolarizability for Polyacetylenes. D. Lu, B. Marten, M. Ringnalda, R. A. Friesner, and W. A. Goddard III. *Chem. Phys. Lett*. **257**, 224 (1996).

D. Semiconductors

D.1. Chemisorbed Species on Semiconductors

82-The Peroxy Radical Model for the Chemisorption of O_2 Onto Silicon Surfaces. W. A. Goddard III, A. Redondo, and T. C. McGill. *Solid State Commun*. **18**, 981 (1976).

120-Theoretical Studies of Si and GaAs Surfaces and Initial Steps in the Oxidation. W. A. Goddard III, J. J. Barton, A. Redondo, and T. C. McGill. *J. Vac. Sci. Technol*. **15**, 1274 (1978).

130-Reconstruction and Oxidation of the GaAs(110) Surface. J. J. Barton, W. A. Goddard III, and T. C. McGill. *J. Vac. Sci. Technol*. **16**, 1178 (1979).

131-Study of Surfaces and Interfaces Using Quantum Chemistry Techniques. W. A. Goddard III and T. C. McGill. *J. Vac. Sci. Technol*. **16**, 1308 (1979).

155-Oxidation of Silicon Surfaces. A. Redondo, W. A. Goddard III, C. A. Swarts, and T. C. McGill. *J. Vac. Sci. Technol*. **19**, 498 (1981).

89-Relaxation of (111) Silicon Surface Atoms from Studies of Si_4H_9 Clusters. A. Redondo, W. A. Goddard III, T. C. McGill, and G. T. Surratt. *Solid State Commun.* **20**, 733 (1976); **21**, 991 (1977).

136-Chemisorption of Oxygen and Aluminum on the GaAs (110) Surface from Ab Initio Theory. J. J. Barton, C. A. Swarts, W. A. Goddard III, and T. C. McGill. *J. Vac. Sci. Technol*. **17**, 164 (1980).

142-Chemisorption of Al and Ga on the GaAs(110) Surface. C. A. Swarts, J. J. Barton, W. A. Goddard III, and T. C. McGill. *J. Vac. Sci. Technol*. **17**, 869 (1980).

194-Donor−Acceptor Oxo Bonds to N, P, As, and Sb States of III-V Semiconductors. R. Chang and W. A. Goddard III. *Surf. Sci.* **149**, 341 (1985).

340-The Surface-Radical Surface−Olefin Recombination Step for CVD Growth of Diamond. Calculation of the Rate Constant from First Principles. C. B. Musgrave, S. J. Harris, and W. A. Goddard III. *Chem. Phys. Lett*. **247**, 359 (1996).

359-Nonthermally Accessible Phase for CO on the Si(100) Surface. D. Hu, W. Ho, X. Chen, S. Wang, and W. A. Goddard III. *Phys. Rev. Lett.* **78**, 1178 (1997).

D.2. Surface Reconstruction of Semiconductors

143-Theoretical Studies of the Reconstruction of the (110) Surface of III-V and II-VI Semiconductor Compounds. C. A. Swarts, W. A. Goddard III, and T. C. McGill. *J. Vac. Sci. Technol*. **17**, 982 (1980).

157-Reconstruction of the (110) Surface of III-V Semiconductor Compounds. C. A. Swarts, T. C. McGill, and W. A. Goddard III. *Surf. Sci.* **110**, 400 (1981).

189-Reconstruction of the (110) Surfaces for III-V Semiconductors; Five Systems Involving In or Sb. R. Chang and W. A. Goddard III. *Surf. Sci.* **144**, 311 (1984).

154-Core to Surface Excitations on GaAs(110). C. A. Swarts, W. A. Goddard III, and T. C. McGill. *J. Vac. Sci. Technol*. **19**, 360 (1981).

156-Geometry of the Abrupt (110) Ge/GaAs Interface. C. A. Swarts, W. A. Goddard III, and T. C. McGill. *J. Vac. Sci. Technol*. **19**, 551 (1981).

159-Electronic Structure of Steps on (111) Silicon Surfaces from Theoretical Studies of Finite Clusters. A. Redondo, W. A. Goddard III, and T. C. McGill. *Phys. Rev. B* **24**, 6135 (1981).

170-Summary Abstract: Mott Insulator Model of the Si(111)-(2×1) Surface. A. Redondo, W. A. Goddard III, and T. C. McGill. *J. Vac. Sci. Technol*. **21**, 328 (1982).

172-Mott Insulator Model of the Si(111)-(2×1) Surface. A. Redondo, W. A. Goddard III, and T. C. McGill. *J. Vac. Sci. Technol*. **21**, 649 (1982).

178-The Mott Insulator Model of the Si(111)-(2×1) Surface. A. Redondo, W. A. Goddard III, and T. C. McGill. *Surf. Sci.* **132**, 49 (1983).

171-Electronic Correlation and the Si(100) Surface: Buckling Versus Nonbuckling. A. Redondo and W. A. Goddard III. *J. Vac. Sci. Technol*. **21**, 344 (1982).

D.3. Defects in Solids

101-The Neutral Vacancy in Silicon and Diamond: Generalized Valence Bond Studies. G. T. Surratt and W. A. Goddard III. *Solid State Commun.* **22**, 413 (1977).

121-Electronic States of Silicon Vacancy: I. Covalent States. G. T. Surratt and W. A. Goddard III. *Phys. Rev. B* **18**, 2831 (1978).

E. Surfaces and Tribology

E.1. Scanning Tunneling Microscopy

270-Scanning Tunneling Microscopy of DNA−Atom-Resolved Imaging, General Observations and Possible Contrast Mechanism. M. G. Youngquist, R. J. Driscoll, T. R. Coley, W. A. Goddard III, and J. D. Baldeschwieler. *J. Vac. Sci. Technol. B* **9**, 1304 (1991).

271-Theoretical Interpretation of Scanning Tunneling Microscopy Images: Application to the Molybdenum-Disulfide Family of Transition-Metal Dichalcogenides. T. R. Coley, W. A. Goddard III, and J. D. Baldeschwieler. *J. Vac. Sci. Technol. B* **9**, 470 (1991).

367-Theoretical Description of the STM Images of Alkanes and Substituted Alkanes Adsorbed on Graphite. F. Faglioni, C. L. Claypool, N. S. Lewis, and W. A. Goddard III. *J. Phys. Chem. B* **101**, 5996 (1997).

368-Source of Image Contrast in STM Images of Functionalized Alkanes on Graphite: A Systematic Functional Group Approach. C. L. Claypool, F. Faglioni, W. A. Goddard III, H. B. Gray, N. S. Lewis, and R. A. Marcus. *J. Phys. Chem. B* **101**, 5978 (1997).

417-Tunneling Mechanism Implications from a Scanning Tunneling Microscopy Study of $H_3C(CH_2)_{15}HC{=}C{=}CH(CH_2)_{15}$-$CH_3$ on Graphite and $C_{14}H_{29}OH$ on MoS_2. C. L. Claypool, F. Faglioni, W. A. Goddard III, and N. S. Lewis. *J. Phys. Chem. B* **103**, 7077 (1999).

423-Effects of Molecular Geometry on the STM Image Contrast of Methyl- and Bromo-Substituted Alkanes and Alkanols on Graphite. C. L. Claypool, F. Faglioni, A. J. Matzger, W. A. Goddard III, and N. S. Lewis. *J. Phys. Chem. B* **103**, 9690 (1999).

E.2. Corrosion

350-The Self-Assembled Monolayer Mechanism of Corrosion Inhibition for Iron Surfaces. S. Ramachandran, B. L. Tsai, M. Blanco, H. J. Chen, Y. Tang, and W. A. Goddard III. In *New Techniques for Characterizing Corrosion and Stress Corrosion*; R. H. Jones and D. R. Baer, Eds. (The Minerals, Metals & Materials Society, 1996); p 117.

355-Self-Assembled Monolayer Mechanism for Corrosion Inhibition of Iron by Imidazolines. S. Ramachandran, B.-L. Tsai, M. Blanco, H. Chen, Y. Tang, and W. A. Goddard III. *Langmuir* **12**, 6419 (1996).

356-Atomistic Simulations of Oleic Imidazolines Bound to Ferric Clusters. S. Ramachandran, B.-L. Tsai, M. Blanco, H. Chen, Y. Tang, and W. A. Goddard III. *J. Phys. Chem*. **101**, 83 (1997).

E.3. Scale

376-Activated Complex Theory of Barite Scale Control Processes. M. Blanco, Y. Tang, P. Shuler, and W. A. Goddard III. *J. Mol. Eng*. **7**, 491 (1997).

E.4. Tribology

351-Structures, Vibrations, and Force Fields of Dithiophosphate Wear Inhibitors from Ab Initio Quantum Chemistry. S. Jiang, S. Dasgupta, M. Blanco, R. Frazier, E. S. Yamaguchi, Y. Tang, and W. A. Goddard III. *J. Phys. Chem*. **100**, 15760 (1996).

372-The SAM Model for Wear Inhibitor Performance of Dithiophosphates on Iron Oxide. S. Jiang, R. Frazier, E. S. Yamaguchi, M. Blanco, S. Dasgupta, Y. Zhou, T. Cagin, Y. Tang, and W. A. Goddard III. *J. Phys. Chem. B* **101**, 7702 (1997).

408-Simulation and Experiments on Friction and Wear of Diamond: A Materials for MEMS and NEMS Application. T. Cagin, J. Che, M. N. Gardos, A. Fijany, and W. A. Goddard III. *Nanotechnology* **10**, 278 (1999).

411-Simulation of Thermal Stability and Friction: A Lubricant Confined Between Monolayers of Wear Inhibitors on Iron Oxide. T. Cagin, Y. Zhou, E. S. Yamaguchi, R. Frazier, A. Ho, Y. Tang, and W. A. Goddard III. *Mater. Res. Soc. Symp. Proc*. **543**, 79 (1999).

F. Metals

F.1. Bonding in Bulk Metals

201-New Concepts of Bonding in Nonperiodic Metallic Systems. M. H. McAdon and W. A. Goddard III. *J. Non-Cryst. Solids* **75**, 149 (1985).

202-New Concepts of Metallic Bonding Based on Valence Bond Ideas. M. H. McAdon and W. A. Goddard III. *Phys. Rev. Lett*. **55**, 2563 (1985).

218-Generalized Valence Bond Studies of Metallic Bonding: Naked Clusters and Applications to Bulk Metals. M. H. McAdon and W. A. Goddard III. *J. Phys. Chem*. **91**, 2607 (1987).

230-Charge Density Waves, Spin Density Waves, and Peierls Distortions in One-Dimensional Metals: I. Hartree−Fock Studies of Cu, Ag, Au, Li, and Na. M. H. McAdon and W. A. Goddard III. *J. Chem. Phys*. **88**, 277 (1988).

235-Charge Density Waves, Spin Density Waves, and Peierls Distortions in One-Dimensional Metals. 2. Generalized Valence Bond Studies of Cu, Ag, Au, Li, and Na. M. H. McAdon and W. A. Goddard III. *J. Phys. Chem*. **92**, 1352 (1988).

254-Interstitial-Electron Model for Lattice Dynamics in fcc Metals. M. Li and W. A. Goddard III. *Phys. Rev. B* **40**, 12155 (1989).

289-Phenomenological Many-Body Potentials from the Interstitial Electron Model. I. Dynamic Properties of Metals. M. Li and W. A. Goddard III. *J. Chem. Phys*. **98**, 7995 (1993).

P51-The Quantum Sutton−Chen Many-Body Potential for Properties of fcc Metals. Y. Kimura, Y. Qi, T. Cagin, and W. A. Goddard III. *Phys. Rev. B*, submitted

F.2. Metallic Alloys

396-Molecular Dynamics Simulations of Glass Formation and Crystallization in Binary Liquid Metals: Cu−Ag and Cu−Ni. Y. Qi, T. Cagin, Y. Kimura, and W. A. Goddard III. *Phys. Rev. B* **59**, 3527 (1999).

404-Strain Rate Induced Amorphization in Metallic Nanowires. H. Ikeda, Y. Qi, T. Cagin, K. Samwer, W. L. Johnson, and W. A. Goddard III. *Phys. Rev. Lett*. **82**, 2900 (1999).

419-Calculation of Mechanical Thermodynamic and Transport Properties of Metallic Glass Formers. T. Cagin, Y. Kimura, Y. Qi, H. Li, H. Ikeda, W. J. Johnson, and W. A. Goddard III. *Mater. Res. Soc. Symp. Proc.* **554**, 43 (1999).

420-Deformation Behavior of fcc Crystalline Metallic Nanowires Under High Strain Rates. Y. Qi, H. Ikeda, T. Cagin, K. Samwer, W. L. Johnson, and W. A. Goddard III. *Mater. Res. Soc. Symp. Proc.* **554**, 367 (1999).

G. Ceramics

G.1. Ceramics

204-Optical Spectrum and Jahn−Teller Splitting of Cu^{++} Sites in K_2CuF_4 Based on Ab Initio Studies of $[CuF_6]^{4-}$ Clusters. S. Yu. Shashkin and W. A. Goddard III. *Phys. Rev. B* **33**, 1353 (1986).

279-The Hessian Biased Force Field for Silicon Nitride Ceramics; Predictions of Thermodynamic and Mechanical Properties for α- and β-Si_3N_4. J. A. Wendel and W. A. Goddard III. *J. Chem. Phys*. **97**, 5048 (1992).

321-Is Carbon Nitride Harder than Diamond? No, But Its Girth Increases When Stretched (Negative Poisson Ratio). Y. Guo and W. A. Goddard III. *Chem. Phys. Lett.* **237**, 72 (1995).

381-Pressure Induced Phase Transformations in Silica. T. Cagin, E. Demiralp, and W. A. Goddard III. In *Microscopic Simulation of Interfacial Phenomena in Solids and Liquid, Materials Research Society Symposium Series 492*; S. R. Phillpot, P. D. Bristowe, D. G. Stround, and J. R. Smith, Eds. (Materials Research Society, 1998); p 287.

384-New Interatomic Potentials for Silica. E. Demiralp, T. Cagin, N. T. Huff, and W. A. Goddard III. *XVII International Congress on Glass, Proceedings*; M. K. Choudhary, N. T. Huff, and C. H. Drummond III, Eds. (1988); p 11.

385-Factors Affecting Molecular Dynamics Simulated Vitreous Silica Structures. N. T. Huff, E. Demiralp, T. Cagin, and W. A. Goddard III. *XVII International Congress on Glass, Proceedings*; M. K. Choudhary, N. T. Huff, and C. H. Drummond III, Eds. (1988); p 61.

399-Theoretical Studies on VPI-5. 3. The MS-Q Force Field for Aluminophosphate Zeolites. O. Kitao, E. Demiralp, T. Cagin, S. Dasgupta, M. Mikami, K. Tanabe, and W. A. Goddard III. *Comput. Mater. Sci*. **14**, 135 (1999).

401-Morse Stretch Potential Charge Equilibrium Force Field for Ceramics: Application to the Quartz−Stishovite Phase Transition and to Silica Glass. E. Demiralp, T. Cagin, and W. A. Goddard III. *Phys. Rev. Lett*. **82**, 1708 (1999).

415-Factors Affecting Molecular Dynamics Simulated Vitreous Silica Structures. N. T. Huff, E. Demiralp, T. Cagin, and W. A. Goddard III, *J. Non-Cryst. Solids* **253**, 133 (1999).

424-Phase Diagram of MgO from Density-Functional Theory and Molecular Dynamics Simulations. A. Strachan, T. Cagin, and W. A. Goddard III *Phys. Rev.* **60**, 15084 (1999).

H. Carbon

H.1. Fullerenes and Fullerene Nanotubes

268-Prediction of Fullerene Packing in C_{60} and C_{70} Crystals. Y. Guo, N. Karasawa, and W. A. Goddard III. *Nature* **351**, 464 (1991).

302-Catalytic Synthesis of Single-Layer Carbon Nanotubes with a Wide Range of Diameters. C-H. Kiang, W. A. Goddard III, R. Beyers, J. R. Salem, and D. S. Bethune. *J. Phys. Chem*. **98**, 6612 (1994).

328-Effects of Catalyst Promoters on the Growth of Single-Layer Carbon Nanotubes. C.-H. Kiang, W. A. Goddard III, R. Beyers, J. R. Salem, and D. S. Bethune. *Mater. Res. Soc. Symp. Proc.* **359**, 69 (1995).

329-Carbon Nanotubes with Single-Layer Walls. C.-H. Kiang, W. A. Goddard III, and D. S. Bethune. *Carbon* **33**, 903 (1995).

331-Catalytic Effects on Heavy Metals on the Growth of Carbon Nanotubes and Nano-particles. C.-H. Kiang, W. A. Goddard III, R. Beyers, J. R. Salem, and D. S. Bethune. *J. Phys. Chem. Solids* **57**, 35 (1995).

344-Structural Modification of Single-Layer Carbon Nanotubes with an Electron Beam. C.-H. Kiang, W. A. Goddard III, R. Beyers, and D. S. Bethune. *J. Phys. Chem*. **100**, 3749 (1996).

354-Novel Structures from Arc-Vaporized Carbon and Metals: Single-Layer Carbon Nanotubes and Metallofullerenes. C.-H. Kiang, P. H. M. van Loosdrecht, R. Beyers, J. R. Salem, D. S. Bethune, W. A. Goddard III, H. C. Dorn, P. Burbank, and S. Stevenson. *Surf. Rev. Lett*. **3**, 765 (1996).

345-Polyyne Ring Nucleus Growth Model for Single-Layer Carbon Nanotubes. C.-H. Kiang and W. A. Goddard III. *Phys. Rev. Lett*. **76**, 2515 (1996).

383-Position of K Atoms in Doped Single-Walled Carbon Nanotube Crystals. G. Gao, T. Cagin, and W. A. Goddard III. *Phys. Rev. Lett*. **80**, 5556 (1998).

390-Energetics, Structure, Mechanical, and Vibrational Properties of Single-Walled Carbon Nanotubes. G. Gao, T. Cagin, and W. A. Goddard III. *Nanotechnology* **9**, 184 (1998).

414-Studies of Fullerenes and Carbon Nanotubes by an Extended Bond Order Potential. J. Che, T. Cagin, and W. A. Goddard III. *Nanotechnology* **10**, 263 (1999).

I. Nanotechnology and Self-Assembly

I.1. Nanotechnology

269-Theoretical Studies of Hydrogen Abstraction Tool for Nanotechnology. C. B. Musgrave, J. K. Perry, R. C. Merkle, and W. A. Goddard III. *Nanotechnology* **2**, 187 (1991).

310-Resonant Tunneling Through Quantum-Dot Arrays. Guanlong Chen, G. Klimeck, S. Datta, Guanhua Chen, and W. A. Goddard III. *Phys. Rev. B* **50**, 8035 (1994).

249-Research Opportunities on Clusters and Cluster-Assembled Materials—A Department of Energy, Council on Materials Science Panel Report; R. P. Andres, R. S. Averback, W. L. Brown, L. E. Brus, W. A. Goddard III, A. Kaldor, S. G. Louie, M. Moscovits, P. S. Peercy, S. J. Riley, R. W. Siegel, F. Spaepen, and Y. Wang. *J. Mater. Res*. **4**, 704 (1989).

391-Molecular Mechanics and Molecular Dynamics Analysis of Drexler−Merkle Gears and Neon Pump. T. Cagin, A. Jaramillo-Botero, G. Gao, and W. A. Goddard III. *Nanotechnology* **9**, 143 (1998).

409-Computational Materials Chemistry at the Nanoscale. T. Cagin, J. Che, Y. Qi, Y. Zhou, E. Demiralp, G. Gao, and W. A. Goddard III. *J. Nanoparticle* **1**, 51 (1999).

418-Diamond and Polycrystalline Diamond for MEMS Applications: Simulations and Experiments. T. Cagin, J. Che, M. N. Gardos, and W. A. Goddard III. *Mater. Res. Soc. Symp. Proc*. **546**, 109 (1999).

I.2. Self-Assembled Monolayers

343-Atomistic Structure for Self-Assembled Monolayers of Alkanethiols on Au(111) Surfaces. J. Gerdy and W. A. Goddard III. *J. Am. Chem. Soc*. **118**, 3233 (1996).

I.3. Nucleation and Phase Transitions

318-Free Energy and Surface Tension of Arbitrarily Large Mackay Icosahedral Clusters. R. B. McClurg, R. C. Flagan, and W. A. Goddard III. *J. Chem. Phys*. **102**, 3322 (1995).

349-Thermodynamic Properties and Homogeneous Nucleation Rates for Surface-Melted Physical Clusters. R. B. McClurg, R. C. Flagan, and W. A. Goddard III. *J. Chem. Phys*. **105**, 7648 (1996).

364-Influences of Binding Transitions on the Homogeneous Nucleation of Mercury. R. B. McClurg, R. C. Flagan, and W. A. Goddard III. In *NanoStructured Materials* (Elsevier Science Ltd., 1997); Vol. 9, pp 53−61.

352-Evidence of Hexatic Phase Formation in Two-Dimensional Lennard-Jones Binary Arrays. M. Li, W. L. Johnson, and W. A. Goddard III. *Phys. Rev.* **54**, 67 (1996).

J. Physical Processes

J.1. Electron Scattering

31-Group Theoretical Selection Rules for Electron-Impact Spectroscopy. W. A. Goddard III, D. L. Huestis, D. C. Cartwright, and S. Trajmar. *Chem. Phys. Lett*. **11**, 329 (1971).

47-The Theoretical Description of an Asymmetric, Nonresonant Charge Transfer Process; $Li + Na^+ \leftrightarrow Li^+ + Na$. The Two-State Approximation. C. F. Melius and W. A. Goddard III. *Chem. Phys. Lett*. **15**, 524 (1972).

49-Theoretical Studies of Nonresonant Charge-Transfer Processes Using a Multistate Molecular Wavefunctions Approach: $Li + Na^+ \leftrightarrow Li^+ + Na$. C. F. Melius and W. A. Goddard III. *Phys. Rev. Lett*. **29**, 975 (1972).

64-Charge Transfer Process Using the Molecular Wavefunction Approach: The Asymmetric Charge Transfer and Excitation in $Li + Na^+$ and $Na + Li^+$. C. F. Melius and W. A. Goddard III. *Phys. Rev. A* **10**, 1541 (1974).

219-Theoretical Studies of Electron Transfer in Metal Dimers: $XY^+ \rightarrow X^+Y$, where X,Y = Be, Mg, Ca, Zn, Cd. R. J. Cave, D. V. Baxter, W. A. Goddard III, and J. D. Baldeschwieler. *J. Chem. Phys*. **87**, 926 (1987).

J.2. Photon Processes

109-The Photodetachment Cross Section of the Negative Hydrogen Ion. M. A. C. Nascimento and W. A. Goddard III. *Phys. Rev. A* **16**, 1559 (1977).

260-Prospects for the Involvement of Transition Metals in the Chemistry of Diffuse Interstellar Clouds: Formation of FeH^+ by Radiative Association. K. K. Irikura, W. A. Goddard III, and J. L. Beauchamp. *Int. J. Mass Spectrom. Ion Processes* **99**, 213 (1990).

266-Photoinitiated H-Atom Reactions in CO_2−HBr Complexes. S. K. Shin, C. Wittig, and W. A. Goddard III. *J. Phys. Chem*. **95**, 8048 (1991).

K. Superconductivity

K.1. Superconductivity in Copper Oxides (High T_c)

233-Electronic Structure and Valence Bond Band Structure of Cuprate Superconducting Materials. Y. Guo, J.-M. Langlois, and W. A. Goddard III. *Science* **239**, 896 (1988).

232-The Magnon Pairing Mechanism of Superconductivity in Cuprate Ceramics. G. Chen and W. A. Goddard III. *Science* **239**, 899 (1988).

247-The Superconducting Properties of Copper Oxide High Temperature Superconductors. G. Chen, J.-M. Langlois, Y. Guo, and W. A. Goddard III. *Proc. Natl. Acad. Sci. U.S.A.* **86**, 3447 (1989).

267-The Quantum Chemistry View of High Temperature Superconductors. W. A. Goddard III, Y. Guo, G. Chen, H. Ding, J-M. Langlois, and G. Lang. In *High Temperature Superconductivity, Proceedings of the 39th Scottish Universities Summer School in Physics*, St. Andrews, Scotland; D. P. Tunstall, W. Barford, and P. Osborne, Eds., 1991.

283-The Band Structure, Magnetic Fluctuations, and Quasiparticle Nature of the Two-Dimensional Three-Band Hubbard Model. H-Q. Ding, G. H. Lang, and W. A. Goddard III. *Phys. Rev. B* **46**, 14317 (1992).

284-Elementary Excitations for the Two-Dimensional Quantum Heisenberg Antiferromagnet. G. Chen, H.-Q. Ding, and W. A. Goddard III. *Phys. Rev. B* **46**, 2933 (1992).

285-Infinite Range Heisenberg Model and High Temperature Superconductivity. J. Tahir-Kheli and W. A. Goddard III. *Phys. Rev. B* **48**, 13002 (1993).

288-Exact Solution to a Strongly Coupled Hubbard Model in One Dimension for High T_c Superconductors. J. Tahir-Kheli and W. A. Goddard III. *Phys. Rev. B* **47**, 1116 (1993).

290-Spinons and Holons in One-Dimensional Three-Band Hubbard Models for High-Temperature Superconductors. J. Tahir-Kheli and W. A. Goddard III. *Proc. Natl. Acad. Sci. U.S.A.* **90**, 9959 (1993).

294-Spin and Charge Dynamics in a One-Dimensional Two-Band Hubbard Model. H.-Q. Ding and W. A. Goddard III. *Phys. Rev. B* **47**, 1149 (1993).

K.2. Superconductivity in Fullerenes

286-Mechanism of Superconductivity in K_3C_{60}. G. Chen and W. A. Goddard III. *Proc. Natl. Acad. Sci. U.S.A.* **90**, 1350 (1993).

297-Electron−Phonon Interactions and Superconductivity in K_3C_{60}. G. Chen, Y. Guo, N. Karasawa, and W. A. Goddard III. *Phys. Rev. B* **48**, 13959 (1993).

K.3. Superconductivity in Organics

312-Ab Initio and Semiempirical Electronic Structural Studies on Bis(ethylenedithio)tetrathiafulvalene (BEDT−TTF or ET). E. Demiralp and W. A. Goddard III. *J. Phys. Chem*. **98**, 9781 (1994).

324-Prediction of New Donors for Organic Superconductors. E. Demiralp and W. A. Goddard III. *Synth. Met*. **72**, 297 (1995).

332-Electron-Transfer Boat-Vibration Mechanism for Superconductivity in Organic Molecules Based on BEDT−TTF. E. Demiralp, S. Dasgupta, and W. A. Goddard III. *J. Am. Chem. Soc.* **117**, 8154 (1995).

360-MSX Force Field and Vibrational Frequencies for BEDT−TTF (Neutral and Cation). E. Demiralp, S. Dasgupta, and W. A. Goddard III. *J. Phys. Chem*. **101**, 1975 (1997).

373-Structures and Energetics Study of Tetrathiafulvalene-Based Donors of Organic Superconductors. E. Demiralp and W. A. Goddard III. *J. Phys. Chem*. *A* **101**, 8128 (1997).

374-Conduction Properties of the Organic Superconductor κ-(BEDT−TTF)$_2$Cu(NCS)$_2$ Based on Hubbard−Unrestricted-Hartree−Fock Band Calculations. E. Demiralp and W. A. Goddard III. *Phys. Rev. B* **56**, 907 (1997).

377-Vibrational Analysis and Isotope Shifts of BEDT−TTF Donor for Organic Superconductors. E. Demiralp and W. A. Goddard III. *J. Chem. Phys*. **102**, 2466 (1998).

L. Atoms and Small Molecules

L.1. Atoms

3-Magnetic Hyperfine Structure of Lithium. W. A. Goddard III. *Phys. Rev.* **157**, 93 (1967).

5-Wavefunctions and Correlation Energies for Two-, Three-, and Four-Electron Atoms. W. A. Goddard III. *J. Chem. Phys*. **48**, 1008 (1968).

6-New Type of Wave Function for Li, Be^+, and B^{++}. W. A. Goddard III. *Phys. Rev.* **169**, 120 (1968).

8-Concerning the Stability of the Negative Ions H^- and Li^-. W. A. Goddard III. *Phys. Rev.* **172**, 7 (1968).

10-Magnetic Hyperfine Structure and Core Polarization in the Excited States of Lithium. W. A. Goddard III. *Phys. Rev.* **176**, 106 (1968).

14-Core Polarization and Hyperfine Structure of the B, C, N, O, and F Atoms. W. A. Goddard III. *Phys. Rev.* **182**, 48 (1969).

30-The Effect of Symmetry Restrictions upon the Hyperfine Properties. P. J. Hay and W. A. Goddard III. *Chem. Phys. Lett*. **9**, 356 (1971).

141-Ab Initio Studies of the X-ray Absorption Edge in Copper Complexes: I. Atomic Cu^{2+} and $Cu(II)Cl_2$. R. A. Bair and W. A. Goddard III. *Phys. Rev. B* **22**, 2767 (1980).

L.2. Ground States of Molecules

13-Electronic Structure of LiH According to a Generalization of the Valence-Bond Method. W. E. Palke and W. A. Goddard III. *J. Chem. Phys*. **50**, 4524 (1969).

27-Spin-Generalized SCF Wavefunctions for H_2O, OH, and O. S. L. Guberman and W. A. Goddard III. *J. Chem. Phys*. **53**, 1803 (1970).

25-A New Type of Wavefunction for BH. R. J. Blint, W. A. Goddard III, R. C. Ladner, and W. E. Palke. *Chem. Phys. Lett*. **5**, 302 (1970).

86-The Nature of the Bonding of Li^+ to H_2O and NH_3: Ab Initio Studies. R. L. Woodin, F. A. Houle, and W. A. Goddard III. *Chem. Phys*. **14**, 461 (1976).

104-Theoretical Studies of CH_3, CH_3^+, and CH_3^- Using Correlated Wavefunctions. G. T. Surratt and W. A. Goddard III. *Chem. Phys*. **23**, 39 (1977).

137-Thermochemistry of *trans*-Diimide and 1,1-Diazene. Ab Initio Studies. C. J. Casewit and W. A. Goddard III. *J. Am. Chem. Soc*. **102**, 4057 (1980).

173-Alkali Oxide Diatomics: Explanation of the Change in Ground State Symmetry from LiO ($^2\Pi$) to CsO ($^2\Sigma^+$). J. N. Allison and W. A. Goddard III. *J. Chem. Phys*. **77**, 4259 (1982).

183-Alkali Oxides. Analysis of Bonding and Explanation of the Reversal in Ordering of the $^2\Pi$ and $^2\Sigma^+$ States. J. N. Allison, R. J. Cave, and W. A. Goddard III. *J. Phys. Chem*. **88**, 1262 (1984).

187-Theoretical Studies on 1,4,6,9-Spiro[4.4]nonatetrayl, an Organic Tetraradical. L. McElwee-White, W. A. Goddard III, and D. A. Dougherty. *J. Am. Chem. Soc.* **106**, 3461 (1984).

239-The C═C Double Bond of Tetrafluoroethylene. E. A. Carter and W. A. Goddard III. *J. Am. Chem. Soc.* **110**, 4077 (1988).

323-Stabilizing the Boat Conformation of Cyclohexane Rings. S. Dasgupta, Y. Tang, J. M. Moldowan, R. M. K. Carlson, and W. A. Goddard III. *J. Am. Chem. Soc.* **117**, 6532 (1995).

388-Conformational Equilibria of β-Alanine and Related Compounds As Studied by NMR Spectroscopy. F. Gregoire, S. H. Wei, E. W. Streed, K. A. Brameld, D. Fort, L. J. Hanely, J. D. Walls, W. A. Goddard, and J. D. Roberts. *J. Am. Chem. Soc.* **120**, 7537 (1998).

412-Conformations and Barriers of Haloethyl Radicals (CH_2XCH_2, X = F,Cl,Br,I): Ab Initio Studies. H. Ihee, A. H. Zewail, and W. A. Goddard III. *J. Phys. Chem.* A **103**, 6638 (1999).

L.3. Methylene and Carbenes

Paper 35 (1972) reported the first accurate (beyond HF) calculations and obtained a ground triplet state ($^3B_1$) with the first excited state ($^1A_1$) higher by $\Delta E = 10.5$ kcal/mol. At the time, the experimental value was $\Delta E \approx 1$ kcal/mol, but Goddard did not consider it as accurate. In 1975, Lineberger published the first direct measurement, leading to $\Delta E = 19.5$ kcal/mol. In the meantime several other calculations had been reported, mostly in the range $\Delta E = 13-16$ kcal/mol. Paper 105 (1976) reexamined them at a much higher level to obtain $\Delta E = 10.2$ kcal/mol with an accuracy expected of $\sim$1 kcal/mol. Goddard concluded that the experimental spectrum had been misinterpreted (because of hot bands). By this point several other groups had obtained $\Delta E \approx 10-12$ kcal/mol, and other experiments were giving values $\Delta E \approx 6-8$ kcal/mol. Paper 113 used the theoretical results to reexamine the experiment to show that the experiment could be reinterpreted in term of the hot bands to give $\Delta E = 9$ kcal/mol; they published the spectra that Lineberger would see without hot bands. Other experimentalists within a year settled on $\Delta E = 9.2$ kcal/mol. Finally, a couple of years later Lineberger built a new apparatus that eliminated hot bands and got exactly the spectra predicted in ref 113. This settled the controversy, theory won, and various experimentalists paid wag the five bottles of champagne they had bet in 1976 when the controversy was raging.

35-Generalized Valence Bond Wavefunctions for the Low Lying States of Methylene. P. J. Hay, W. J. Hunt, and W. A. Goddard III. *Chem. Phys. Lett.* **13**, 30 (1972).

105-Ab Initio Studies on the Singlet−Triplet Splitting of Methylene (CH_2). L. B. Harding and W. A. Goddard III. *J. Chem. Phys.* **67**, 1777 (1977).

113-Methylene: Ab Initio Vibronic Analysis and Reinterpretation of the Spectroscopic and Negative Ion Photoelectron Experiments. L. B. Harding and W. A. Goddard III. *Chem. Phys. Lett.* **55**, 217 (1978).

61-Comparison of INDO and Ab Initio Methods for Correlated Wave Functions of the Ground and Excited States of Methylene and Ethylene. W. R. Wadt and W. A. Goddard III. *J. Am. Chem. Soc.* **96**, 5996 (1974).

216-Electron Correlation, Basis Sets, and the Methylene Singlet−Triplet Gap. E. A. Carter and W. A. Goddard III. *J. Chem. Phys.* **86**, 862 (1987).

222-New Predictions for Singlet−Triplet Gaps of Substituted Carbenes. E. A. Carter and W. A. Goddard III. *J. Phys. Chem.* **91**, 4651 (1987).

231-Correlation-Consistent Singlet−Triplet Gaps in Substituted Carbenes. E. A. Carter and W. A. Goddard III. *J. Chem. Phys.* **88**, 1752 (1988).

282-Singlet Triplet Gaps in Substituted Carbenes CXY (X, Y = H, F, Cl, Br, I, SiH_3). K. K. Irikura, W. A. Goddard III, and J. L. Beauchamp. *J. Am. Chem. Soc.* **114**, 48 (1992).

L.4. Excited States of Molecules

20-The Theoretical Description of the ($\pi\pi^*$) Excited States of Ethylene. T. H. Dunning, Jr., W. J. Hunt, and W. A. Goddard III. *Chem. Phys. Lett.* **4**, 147 (1969).

44-Multiconfiguration Wavefunctions for the Lowest ($\pi\pi^*$) Excited State of Ethylene. C. F. Bender, T. H. Dunning, Jr., H. F. Schaefer III, W. A. Goddard III, and W. J. Hunt. *Chem. Phys. Lett.* **15**, 171 (1972).

38-Orbital Description of the Excited States of LiH. C. F. Melius and W. A. Goddard III. *J. Chem. Phys.* **56**, 3348 (1972).

39-Theoretical Results for the Excited States of Ozone. P. J. Hay and W. A. Goddard III. *Chem. Phys. Lett.* **14**, 46 (1972).

55-Theoretical Evidence for Bound Electronic Excited States of Ozone. P. J. Hay, T. H. Dunning, Jr., and W. A. Goddard III. *Chem. Phys. Lett.* **23**, 457 (1973).

58-Comparison of INDO and Ab Initio Methods for the Correlated Wave Functions of the Ground and Excited States of Ozone. W. R. Wadt and W. A. Goddard III. *J. Am. Chem. Soc.* **96**, 1689 (1974).

68-Configuration Interaction Studies of O_3 and O_3^+. Ground and Excited States. P. J. Hay, T. H. Dunning, Jr., and W. A. Goddard III. *J. Chem. Phys.* **62**, 3912 (1975).

106-Ab Initio Theoretical Results on the Stability of Cyclic Ozone. L. B. Harding and W. A. Goddard III. *J. Chem. Phys.* **67**, 2377 (1977).

52-Theoretical Assignments of the Low-Lying Electronic States of Carbon Dioxide. N. W. Winter, C. F. Bender, and W. A. Goddard III. *Chem. Phys. Lett.* **20**, 489 (1973).

54-Theoretical and Experimental (Electron Impact) Studies of the Low-Lying Rydberg States in O_2. D. C. Cartwright, W. J. Hunt, W. Williams, S. Trajmar, and W. A. Goddard III. *Phys. Rev. A* **8**, 2436 (1973).

76-Configuration Interaction Studies on Low-Lying States of O_2. B. J. Moss and W. A. Goddard III. *J. Chem. Phys.* **63**, 3523 (1975).

57-The Rydberg Nature and Assignments of Excited States of the Water Molecule. W. A. Goddard III and W. J. Hunt. *Chem. Phys. Lett.* **24**, 464 (1974).

72-Configuration Interaction Studies of the Excited States of Water. N. W. Winter, W. A. Goddard III, and F. W. Bobrowicz. *J. Chem. Phys.* **62**, 4325 (1975).

88-The Low-Lying Excited States of Water, Methanol, and Dimethyl Ether. W. R. Wadt and W. A. Goddard III. *Chem. Phys.* **18**, 1 (1976).

66-The Electronic Structure of Pyrazine. A Valence Bond Model for Lone Pair Interactions. W. R. Wadt and W. A. Goddard III. *J. Am. Chem. Soc.* **97**, 2034 (1975).

85-The Electronic Structure of Pyrazine: Configuration Interaction Calculations Using an Extended Basis. W. R. Wadt, W. A. Goddard III, and T. H. Dunning, Jr. *J. Chem. Phys.* **65**, 438 (1976).

69-Dipole Moments and Electric Field Gradients for Correlated Wavefunctions of NO: The X ^2P, A $^2S^+$, and D $^2S^+$ States. S. P. Walch and W. A. Goddard III. *Chem. Phys. Lett.* **33**, 18 (1975).

70-Theoretical Description of the $^2A''$ and $^2A'$ States of the Peroxyformyl Radical. N. W. Winter, W. A. Goddard III, and C. F. Bender. *Chem. Phys. Lett.* **33**, 25 (1975).

167-Ab Initio Studies of the Structure of Peroxides and Peroxy Radicals. R. A. Bair and W. A. Goddard III. *J. Am. Chem. Soc.* **104**, 2719 (1982).

74-The Generalized Valence Bond Description of the Low-Lying States of Diazomethane. S. P. Walch and W. A. Goddard III. *J. Am. Chem. Soc.* **97**, 5319 (1975).

80-Triplet States of the Amide Group: Trapped Electron Spectra of Formamide and Related Molecules. R. H. Staley, L. B. Harding, W. A. Goddard III, and J. L. Beauchamp. *Chem. Phys. Lett*. **36**, 589 (1975).

77-The Generalized Valence Bond Description of the Low-Lying States of Formaldehyde. L. B. Harding and W. A. Goddard III. *J. Am. Chem. Soc.* **97**, 6293 (1975).

94-Ab Initio Theoretical Studies of the Rydberg States of Formaldehyde. L. B. Harding and W. A. Goddard III. *J. Am. Chem. Soc.* **99**, 677 (1977).

78-The Generalized Valence Bond Description of the Valence States of Formamide. L. B. Harding and W. A. Goddard III. *J. Am. Chem. Soc.* **97**, 6300 (1975).

87-The Generalized Valence Bond Description of the Low-Lying States of Ketene. L. B. Harding and W. A. Goddard III. *J. Am. Chem. Soc.* **98**, 6093 (1976).

91-The Low Lying States of Ammonia: Generalized Valence Bond and Configuration Interaction Studies. R. Rianda, R. P. Frueholz, and W. A. Goddard III. *Chem. Phys.* **19**, 131 (1977).

93-The Theoretical Determination of the B ^1P_u Potential Energy Curve for Li_2. L. R. Kahn, T. H. Dunning, Jr., N. W. Winter, and W. A. Goddard III. *J. Chem. Phys*. **66**, 1135 (1977).

96-Theoretical Studies of the Low-Lying States of Vinylidene. J. H. Davis, W. A. Goddard III, and L. B. Harding. *J. Am. Chem. Soc.* **99**, 2919 (1977).

107-Electronic States of Aminonitrene (1,1-Diazine): A Study of the Endwise Bonding of Dinitrogen. J. H. Davis and W. A. Goddard III. *J. Am. Chem. Soc.* **99**, 7111 (1977).

125-The Excited Electronic States of All-Trans-1,3,5-Hexatriene. M. A. C. Nascimento and W. A. Goddard III. *Chem. Phys. Lett*. **60**, 197 (1979).

126-The Valence Electronic Excited States of trans-1,3-Butadiene and trans,trans-1,3,5-Hexatriene from Generalized Valence Bond and Configuration Interaction Calculations. M. A. C. Nascimento and W. A. Goddard III. *Chem. Phys*. **36**, 147 (1979).

144-The Rydberg States of trans-Butadiene from Generalized Valence Bond and Configuration Interaction Calculations. M. A. C. Nascimento and W. A. Goddard III. *Chem. Phys*. **53**, 251 (1980).

145-The Rydberg States of trans-1,3,5-Hexatriene from Ab Initio and Configuration Interaction Calculations. M. A. C. Nascimento and W. A. Goddard III. *Chem. Phys.* **53**, 265 (1980).

212-The Generalized Resonating Valence Bond Description of Cyclobutadiene. A. F. Voter and W. A. Goddard III. *J. Am. Chem. Soc.* **108**, 2830 (1986).

L.5. Reaction Surfaces

16-Ab Initio Calculations on the $H_2 + D_2 \leftrightarrow 2HD$ Four-Center Exchange Reaction: I. Elements of the Reaction Surface. C. W. Wilson, Jr. and W. A. Goddard III. *J. Chem. Phys*. **51**, 716 (1969).

22-The Optimum Orbitals for the $H_2 + D \leftrightarrow H + HD$ Exchange Reaction. W. A. Goddard III and R. C. Ladner. *Int. J. Quantum Chem*. **IIIS**, 63 (1969).

32-A Generalized Orbital Description of the Reactions of Small Molecules. W. A. Goddard III and R. C. Ladner. *J. Am. Chem. Soc.* **93**, 6750 (1971).

M. Methodology

M.1. Quantum Mechanics. Generalized Valence Bond (GVB)

The Generalized valence bond (GVB) wavefunction is the most general in which the many-body wavefunction can be interpreted in terms of self-consistent independent particles. The original motivation was to develop a method for incorporating electron correlation while retaining the ability to interpret the wavefunction in terms of orbital concepts. This has proved quite useful, leading to a new VB view of bonding that leads to a much better understanding of geometries, properties, and excitation energies of main group and transition metal systems. It also leads to selection rules useful for predicting the reactions of main group and transition metal systems.

Papers 1, 2, 4, 7, and 17 developed the general approach, which was summarized in paper 23. The spin-optimized (SOGI) wave function was later referred to as GVB.

1-Improved Quantum Theory of Many-Electron Systems: I. Construction of Eigenfunctions of S^2 Which Satisfy Pauli's Principle. W. A. Goddard III. *Phys. Rev.* **157**, 73 (1967).

2-Improved Quantum Theory of Many-Electron Systems: II. The Basic Method. W. A. Goddard III. *Phys. Rev.* **157**, 81 (1967).

4-Improved Quantum Theory of Many-Electron Systems: III. The GF Method. W. A. Goddard III. *J. Chem. Phys*. **48**, 450 (1968).

7-Improved Quantum Theory of Many-Electron Systems: IV. Properties of GF Wavefunctions. W. A. Goddard III. *J. Chem. Phys*. **48**, 5337 (1968).

17-Improved Quantum Theory of Many-Electron Systems: V. The Spin-Coupling Optimized GI Method. R. C. Ladner and W. A. Goddard III. *J. Chem. Phys*. **51**, 1073 (1969).

23-The Symmetric Group and the Spin Generalized SCF Method. W. A. Goddard III. *Int. J. Quantum Chem*. **IIIS**, 593 (1970).

M.2. Quantum Mechanics. GVB Perfect Pairing (GVB-PP)

Since GVB allows all orbitals to overlap all other orbitals, the calculations scale with the number of atoms as $N!$. GVB-PP (PP for perfect pairing), developed in papers 43 and 50, is a restricted form of GVB in which only (singlet-paired) pairs of orbitals are allowed to overlap. This leads to practical calculations that scale in the same way as simple Hartree−Fock wave functions. The equations for the general case were developed in papers 19, 21, and 26 and generalized in paper 108. Papers 317 and 298 show how to choose trial functions and how to speed convergence.

43-Self-Consistent Procedures for Generalized Valence Bond Wavefunctions: Applications H_3, BH, H_2O, C_2H_6, and O_2. W. J. Hunt, P. J. Hay, and W. A. Goddard III. *J. Chem. Phys*. **57**, 738 (1972).

50-Generalized Valence Bond Description of Simple Alkanes, Ethylene and Acetylene. P. J. Hay, W. J. Hunt, and W. A. Goddard III. *J. Am. Chem. Soc.* **94**, 8293 (1972).

19-The Orthogonality Constrained Basis Set Expansion Method for Treating Off-Diagonal Lagrange Multipliers in Calculations of Electronic Wave Functions. W. J. Hunt, T. H. Dunning, Jr., and W. A. Goddard III. *Chem. Phys. Lett*. **3**, 606 (1969).

21-The Proper Treatment of Off-Diagonal Lagrange Multipliers and Coupling Operators in Self-Consistent Field Equations. W. A. Goddard III, T. H. Dunning, Jr., and W. J. Hunt. *Chem. Phys. Lett*. **4**, 231 (1969).

26-The Incorporation of Quadratic Convergence into Open-Shell Self-Consistent Field Equations. W. J. Hunt, W. A. Goddard III, and T. H. Dunning, Jr. *Chem. Phys. Lett*. **6**, 147 (1970).

108-The Self-Consistent Field Equations for Generalized Valence Bond and Open-Shell Hartree−Fock Wavefunctions. F. W. Bobrowicz and W. A. Goddard III. In *Modern Theoretical Chemistry: Methods of Electronic Structure Theory*; H. F. Schaefer III, Ed. (Plenum Press, NY, 1977); Vol. 3, Chapter 4, pp 79−127.

317-Rule-Based Trial Wavefunctions for Generalized Valence Bond Theory. J.-M. Langlois, T. Yamasaki, R. P. Muller, and W. A. Goddard III. *J. Phys. Chem*. **98**, 13498 (1994).

298-A Generalized Direct Inversion of the Iterative Subspace Approaches for Generalized Valence Bond Wavefunctions (GVB-DIIS). R. P. Muller, J.-M. Langlois, M. N. Ringnalda, R. A. Friesner, and W. A. Goddard III. *J. Chem. Phys*. **100**, 1226 (1994).

M.3. Quantum Mechanics. GVB-PP plus Spin Coupling

The biggest difference between GVB-PP and full GVB is the lack of spin couplings other than perfect pairing. The most practical way to do this is GVB-RCI (RCI for restricted CI), which allowed all spin couplings between the occupied orbitals but did not reoptimize them (see papers 35, 76, 77 for applications). Paper 79 showed how to optimize spin coupling within the PP framework. Paper 83 developed general equations for optimizing the orbitals for GVB-RCI wavefunctions. Paper 309 developed a more practical method for optimizing the orbitals of GVB-RCI that did not require full integral transformations.

79-The Generalized Valence Bond Description of O_2. B. J. Moss, F. W. Bobrowicz, and W. A. Goddard III. *J. Chem. Phys*. **63**, 4632 (1975).

83-Orbital Optimization in Electronic Wavefunctions; Equations for Quadratic and Cubic Convergence in General Multiconfiguration Wavefunctions. L. G. Yaffe and W. A. Goddard III. *Phys. Rev. A* **13**, 1682 (1976).

309-Pseudospectral Contracted Configuration Interaction from a Generalized Valence Bond Reference. R. B. Murphy, R. A. Friesner, M. N. Ringnalda, and W. A. Goddard III. *J. Chem. Phys*. **101**, 2986 (1994).

403-GVB-RP: A Reliable MCSCF Wave Function for Large Systems. F. Faglioni and W. A. Goddard III. *Int. J. Quantum Chem*. **74**, 1 (1999).

M.4. Quantum Mechanics. Spatial Projection and Resonance

These papers generalize the orbital product form of GVB to handle systems with resonance of equivalent spatial configurations. Spatially projected GVB wave functions were developed in papers 40, 48, 60, 63, and 67. Resonance GVB was developed in papers 151, 158.

48-The Valence Bond Aufbau Principle for Molecular Excited States. D. L. Huestis and W. A. Goddard III. *Chem. Phys. Lett*. **16**, 157 (1972).

40-On the Origin of Energy Barriers in the Excited States of He_2. S. L. Guberman and W. A. Goddard III. *Chem. Phys. Lett*. **14**, 460 (1972).

75-Nature of the Excited States of He_2. S. L. Guberman and W. A. Goddard III. *Phys. Rev. A* **12**, 1203 (1975).

60-The Generalized Valence Bond π Orbitals of Ethylene and Allyl Cation. G. Levin, W. A. Goddard III, and D. L. Huestis. *Chem. Phys.* **4**, 409 (1974).

65-The Generalized Valence Bond Description of Allyl Radical. G. Levin and W. A. Goddard III. *J. Am. Chem. Soc.* **97**, 1649 (1975).

67-Spatially Projected Generalized Valence Bond Description of the pi-States of Allyl Radical. G. Levin and W. A. Goddard III. *Theor. Chim. Acta* **37**, 253 (1975).

151-A Method for Describing Resonance Between Generalized Valence Bond Wavefunctions. A. F. Voter and W. A. Goddard III. *Chem. Phys.* **57**, 253 (1981).

158-The Generalized Resonating Valence Bond Method: Barrier Heights in the HF + D and HCl + D Exchange Reactions. A. F. Voter and W. A. Goddard III. *J. Chem. Phys*. **75**, 3638 (1981).

316-Parallel Calculation of Electron-Transfer and Resonance Matrix Elements of Hartree−Fock and Generalized Valence Bond Wavefunctions. E. P. Bierwagen, T. R. Coley, and W. A. Goddard III. *ACS Symposium Series 592, Parallel Computing in Computational Chemistry*; T. G. Mattson Ed. (American Chemical Society, Washington DC, 1995); Chapter 7, p 84.

M.5. Pseudospectral GVB

257-Pseudospectral Generalized Valence Bond Calculations: Application to Methylene, Ethylene, and Silylene. J.-M. Langlois, R. P. Muller, T. R. Coley, W. A. Goddard III, and M. N. Ringnalda. *J. Chem. Phys*. **92**, 7488 (1990).

314-Accurate First Principles Calculation of Molecular Charge Distributions and Solvation Energies from Ab Initio Quantum Mechanics and Continuum Dielectric Theory. D. J. Tannor, B. Marten, R. Murphy, R. A. Friesner, D. Sitkoff, A. Nicholls, M. Ringnalda, W. A. Goddard III, and B. Honig. *J. Am. Chem. Soc.* **116**, 11875 (1994).

315-New Pseudospectral Algorithms for Electronic Structure Calculations: Length Scale Separation and Analytical Two-Electron Integral Corrections. B. H. Greeley, T. V. Russo, D. T. Mainz, R. A. Friesner, J.-M. Langlois, W. A. Goddard III, R. E. Donnelly, and M. N. Ringnalda. *J. Chem. Phys*. **101**, 4028 (1994).

M.6. Configuration Interaction Methods

15-Excited States of H_2O Using Improved Virtual Orbitals. W. J. Hunt and W. A. Goddard III. *Chem. Phys. Lett*. **3**, 414 (1969).

237-Correlation-Consistent Configuration Interaction: Accurate Bond Dissociation Energies from Simple Wavefunctions. E. A. Carter and W. A. Goddard III. *J. Chem. Phys*. **88**, 3132 (1988).

242-Optimized Two-Electron Integral Transformation Procedures for Vector-Concurrent Architectures. J. N. Hurley, D. L. Huestis, and W. A. Goddard III. *J. Phys. Chem*. **92**, 4880 (1988).

M.7. Density Functional Theory

365-Generalized Generalized Gradient Approximation: An Improved Density-Functional Theory for Accurate Orbital Eigenvalues. X. Hua, X. Chen, W. A. Goddard III. *Phys. Rev. B* **55**, 103 (1997).

M.8. Periodic Boundary Conditions

12-Lithium Energy-Band Structure Calculations Using Ab Initio Pseudopotentials. P. M. O'Keefe and W. A. Goddard III. *Phys. Rev.* **180**, 747 (1969).

18-New Approach to Energy-Band Calculations with Results for Lithium Metal. P. M. O'Keefe and W. A. Goddard III. *Phys. Rev. Lett*. **23**, 300 (1969).

29-The Use of the GI Method in Band Calculations on Solids. W. A. Goddard III and P. M. O'Keefe. In *Computational Methods in Band Theory*; P. M. Marcus, J. F. Janak, and A. R. Williams, Eds. (Plenum Press, New York, 1971); pp 542−569.

140-Ab Initio Hartree−Fock Calculations of Crystalline Systems Using Full-Symmetry Analysis of Basis Set Expansions. T. H. Upton and W. A. Goddard III. *Phys. Rev. B* **22**, 1534 (1980).

338-Dual-Space Approach for Density-Functional Calculations of Two- and Three-Dimensional Crystals Using Gaussian

Basis Functions. X. J. Chen, J.-M. Langlois, and W. A. Goddard III. *Phys. Rev. B* **52**, 2348 (1995).

327-First Principles Studies of Band Offsets at Heterojunctions and of Surface Reconstruction Using Gaussian Dual-Space Density Functional Theory. X. Chen, A. Mintz, J. Hu, X. Hua, J. Zinck, and W. A. Goddard III. *J. Vac. Sci. Technol*. **13**, 1715 (1995).

339-Band Structures of II-VI Semiconductors using Gaussian Basis Functions with Separable Ab Initio Pseudopotentials: Application to Prediction of Band Offsets. X. Chen, X. Hua, J. Hu, J.-M. Langlois, and W. A. Goddard III. *Phys. Rev. B* **53**, 1377 (1996).

M.9. Pseudopotentials

Goddard pioneered the development of *ab initio pseudopotentials* or effective core potentials, widely accepted now as a rigorous way to replace core electrons in ab initio calculations. The original idea was in paper 9 (1968), which was tested in papers 11, 36, and 37. The advance of being able to develop ECP from HF wave functions of atoms was developed in paper 63 and applied to transition metals in papers 62. Paper 98 introduced the idea now referred to as a norm-conserving PP and applied it to Si. Paper 150 showed how to include valence Coulomb terms in deriving ECP and reported the ECP for NaCl. Paper 165 reported the ECP for Ga, Ge, As. These approaches were used by Hay and Wadt and by Hamann and Schluter to develop ECP for the whole periodic table and are the standard used in the chemistry and physics communities.

9-New Foundation for the Use of Pseudopotentials in Metals. W. A. Goddard III. *Phys. Rev.* **174**, 659 (1968).

11-A Direct Test of the Validity of the Use of Pseudopotentials in Molecules. L. R. Kahn and W. A. Goddard III. *Chem. Phys. Lett*. **2**, 667 (1968).

36-Ab Initio Effective Potentials for Use in Molecular Calculations. L. R. Kahn and W. A. Goddard III. *J. Chem. Phys*. **56**, 2685 (1972).

37-Use of Ab Initio G1 Effective Potentials for Calculations of Molecular Excited States. C. F. Melius, W. A. Goddard III, and L. R. Kahn. *J. Chem. Phys*. **56**, 3342 (1972).

63-Ab Initio Effective Potentials for Use in Molecular Quantum Mechanics. C. F. Melius and W. A. Goddard III. *Phys. Rev. A* **10**, 1528 (1974).

62-Fe and Ni Ab Initio Effective Potentials for Use in Molecular Calculations. C. F. Melius, B. D. Olafson, and W. A. Goddard III. *Chem. Phys. Lett*. **28**, 457 (1974).

98-Ab Initio Effective Potentials for Silicon. A. Redondo, W. A. Goddard III, and T. C. McGill. *Phys. Rev. B* **15**, 5038 (1977).

150-The Shape and Hamiltonian Consistent (SHC) Effective Potentials. A. K. Rappé, T. A. Smedley, and W. A. Goddard III. *J. Phys. Chem*. **85**, 1662 (1981).

165-Core Effective Potentials for Ga, Ge, and As. J. J. Barton, C. A. Swarts, and W. A. Goddard III. *Phys. Rev.* B **25**, 2812 (1982).

M.10. Force Fields from QM

250-Hessian-Biased Force Fields from Combining Theory and Experiment. S. Dasgupta and W. A. Goddard III. *J. Chem. Phys*. **90**, 7207 (1989).

341-The Hessian Biased Singular Value Decomposition Method for Optimization and Analysis of Force Fields. S. Dasgupta, T. Yamasaki, and W. A. Goddard III. *J. Chem. Phys*. **104**, 2898 (1996).

363-The Hindered Rotor Density-of-States Interpolation Function. R. B. McClurg, R. C. Flagan, and W. A. Goddard III. *J. Chem. Phys*. **106**, 6675 (1997).

M.11. Empirical Force Fields

256-DREIDING: A Generic Force Field for Molecular Simulations. S. L. Mayo, B. D. Olafson, and W. A. Goddard III. *J. Phys. Chem*. **94**, 8897 (1990).

264-Charge Equilibration for Molecular Dynamics Simulations. A. K. Rappé, and W. A. Goddard III. *J. Phys. Chem*. **95**, 3358 (1991).

275-UFF, a Full Periodic Table Force Field for Molecular Mechanics and Molecular Dynamics Simulations. A. K. Rappé, C. J. Casewit, K. S. Colwell, W. A. Goddard III, and W. M. Skiff. *J. Am. Chem. Soc*. **114**, 10024 (1992).

330-Polarization Effects in the AgBr Interactions Potentials. C.-H. Kiang and W. A. Goddard III. *J. Phys. Chem*. **99**, 14334 (1995).

406-Generalized Extended Empirical Bond-order Dependent Force Fields Including Nonbond Interactions. J. Che, T. Cagin, and W. A. Goddard III. *Theor. Chem. Acc*. **102**, 346 (1999).

M.12. Molecular Dynamics Methods

252-Acceleration of Convergence for Lattice Sums. N. Karasawa and W. A. Goddard III. *J. Phys. Chem*. **93**, 7320 (1989).

366-Fast Ewald Sums for General van der Waals Potentials. Z. Chen, T. Cagin, and W. A. Goddard III. *J. Comput. Chem*. **18**, 1365 (1997).

273-Optimal Spline Cutoffs for Coulomb and van der Waals Interactions. H-Q. Ding, N. Karasawa, and W. A. Goddard III. *Chem. Phys. Lett*. **193**, 197 (1992).

272-Atomic Level Simulations on a Million Particles: The Cell Multipole Method for Coulomb and London Nonbond Interactions. H. Q. Ding, N. Karasawa, and W. A. Goddard III. *J. Chem. Phys*. **97**, 4309 (1992).

274-The Reduced Cell Multipole Method for Coulomb Interactions in Periodic Systems with Million-Atom Unit Cells. H. Ding, N. Karasawa, and W. A. Goddard III. *Chem. Phys. Lett*. **196**, 6 (1992).

358-Molecular Dynamics for Very Large Systems on Massively Parallel Computers: The MPSim Program. K-T. Lim, S. Brunett, M. Iotov, R. B. McClurg, N. Vaidehi, S. Dasgupta, S. Taylor, and W. A. Goddard III. *J. Comput. Chem*. **18**, 501 (1997).

265-Canonical Dynamics Simulations of Single-Chain Polyethylene. T. Cagin, W. A. Goddard III, and M. L. Ary. *Comput. Polym. Sci*. **I**, 241 (1991).

287-Effective Hamiltonians for Motions with Disparate Time Scales: The Quantum Shell Model and the Classical Statistical Shell Model. C. H. Kiang and W. A. Goddard III. *J. Chem. Phys*. **98**, 1451 (1993).

348-Constant Temperature Constrained Molecular Dynamics: The Newton−Euler Inverse Mass Operator Method. N. Vaidehi, A. Jain, and W. A. Goddard III. *J. Phys. Chem*. **100**, 10508 (1996).

389-A Fast Algorithm for Massively Parallel, Long-Term, Simulation of Complex Molecular Dynamics Systems. A. Fijany, T. Cagin, A. Jaramillo-Botero, and W. A. Goddard III. In *Parallel Computing: Fundamentals, Applications and New Directions*; E. H. D'Hollander, G. R. Joubert, F. J. Peters, and U. Tottenberg, Eds. (Elsevier Science B.V., 1998); pp 505.

416-Novel Algorithms for Massively Parallel, Long-term, Simulation of Molecular Dynamics Systems. A. Fijany, T. Cagin, A. Jaramillo-Botero, and W. A. Goddard III. *Adv. Eng. Software* **29**, 441 (1998).

M.13. Monte Carlo Methods

244-Phase Transitions in Polymethylene Single Chains from Monte Carlo Simulations. N. Karasawa and W. A. Goddard III. *J. Phys. Chem*. **92**, 5828 (1988).

325-Building Proteins from C_α Coordinates Using the Dihedral Probability Grid Monte Carlo Method. A. M. Mathiowetz and W. A. Goddard III. *Protein Sci*. **4**, 1217 (1995).

326-De novo Prediction of Polypeptide Conformations Using Dihedral Probability Grid Monte Carlo Methodology. J. S. Evans, A. M. Mathiowetz, S. I. Chan, and W. A. Goddard III. *Protein Sci*. **4**, 1203 (1995).

362-The Continuous Configurational Boltzmann Biased Direct Monte Carlo Method for Free Energy Properties of Polymer Chains. J. Sadanobu and W. A. Goddard III. *J. Chem. Phys*. **106**, 6722 (1997).

386-Efficient Monte Carlo Method for Free Energy Evaluation of Polymer Chains. J. Sadanobu and W. A. Goddard III *Fluid Phase Equilib.* **144**, 415 (1998).

N. Interpretation

N.1. Exchange Kinetic Energy View of Bonding

24-Exchange Kinetic Energy, Contragradience, and Chemical Binding. C. W. Wilson, Jr. and W. A. Goddard III. *Chem. Phys. Lett*. **5**, 45 (1970).

41-Ab Initio Calculations on the $H_2 + D_2 \leftrightarrow 2HD$ Four-Center Exchange Reactions: II. Orbitals, Contragradience, and the Reaction Surface. C. W. Wilson, Jr. and W. A. Goddard III. *J. Chem. Phys*. **56**, 5913 (1972).

45-The Role of Kinetic Energy in Chemical Binding: I. The Nonclassical or Exchange Kinetic Energy. C. W. Wilson, Jr. and W. A. Goddard III. *Theor. Chim. Acta* **26**, 195 (1972).

46-The Role of Kinetic Energy in Chemical Binding: II. Contragradience. W. A. Goddard III and C. W. Wilson, Jr. *Theor. Chim. Acta* **26**, 211 (1972).

N.2. GVB Model of Bonding

42-The Generalized Valence Bond View of Molecules; The BH_n Series. W. A. Goddard III and R. J. Blint. *Chem. Phys. Lett*. **14**, 616 (1972).

51-Orbital Description and Properties of the BH Molecule. R. J. Blint and W. A. Goddard III. *J. Chem. Phys*. **57**, 5296 (1972).

59-The Orbital Description of the Potential Energy Curves and Properties of the Lower Excited States of the BH Molecule. R. J. Blint and W. A. Goddard III. *Chem. Phys.* **3**, 297 (1974).

53-Generalized Valence Bond Description of Bonding in Low-Lying States of Molecules. W. A. Goddard III, T. H. Dunning, Jr., W. J. Hunt, and P. J. Hay. *Acc. Chem. Res*. **6**, 368 (1973).

124-The Description of Chemical Bonding from Ab Initio Calculations. W. A. Goddard III and L. B. Harding. *Annu. Rev. Phys. Chem*. **29**, 363 (1978).

198-Intraatomic Exchange and the Violation of Hund's Rule in Twisted Ethylene. A. F. Voter, M. M. Goodgame, and W. A. Goddard III. *Chem. Phys.* **98**, 7 (1985).

209-Relation Between Singlet−Triplet Gaps and Bond Energies. E. A. Carter and W. A. Goddard III. *J. Phys. Chem*. **90**, 998 (1986).

243-Relationships Between Bond Energies in Coordinately Unsaturated and Coordinately Saturated Transition Metal Complexes: A Quantitative Guide for Single, Double, and Triple Bonds. E. A. Carter and W. A. Goddard III. *J. Phys. Chem*. **92**, 5679 (1988).

379-Correction Analysis of Chemical Bond. T. Yamasaki and W. A. Goddard III. *J. Phys. Chem*. **102**, 2919 (1998).

N.3. The GVB Model for Bonding to Transition Metals

208-Theoretical Studies of Transition Metal Hydrides. 1. Bond Energies for MH^+ with M = Ca, Sc, T, V, Cr, Mn, Fe, Co, Ni, Cu, and Zn. J. B. Schilling, W. A. Goddard III, and J. L. Beauchamp. *J. Am. Chem. Soc*. **108**, 582 (1986).

223-Theoretical Studies of Transition Metal Hydrides. 3. SrH^+ through CdH^+. J. B. Schilling, W. A. Goddard III, and J. L. Beauchamp. *J. Am. Chem. Soc.* **109**, 5565 (1987).

224-Theoretical Studies of Transition Metal Methyl Ions, MCH_3^+: M = Sc, Cr, Mn, Zn, Y, Mo, Tc, Pd, and Cd. J. B. Schilling, W. A. Goddard III, and J. L. Beauchamp. *J. Am. Chem. Soc.* **109**, 5573 (1987).

226-Theoretical Studies of Transition Metal Hydrides. 2. CaH^+ through ZnH^+. J. B. Schilling, W. A. Goddard III, and J. L. Beauchamp. *J. Phys. Chem*. **91**, 5616 (1987).

259-Theoretical Study of Transition-Metal Hydrides. 5. HfH^+ through HgH^+, BaH^+, and LaH^+. G. Ohanessian, M. J. Brusich, and W. A. Goddard III. *J. Am. Chem. Soc.* **112**, 7179 (1990).

261-Valence Bond Concepts in Transition Metals: Metal Hydride Diatomic Cations. G. Ohanessian and W. A. Goddard III. *Acc. Chem. Res*. **23**, 386 (1990).

221-Theoretical Studies of Transition Metal Hydrides. 4. Comparison of Transition Metal Dihydride Ions CrH_2^+ and MoH_2^+. J. B. Schilling, W. A. Goddard III, and J. L. Beauchamp. *J. Phys. Chem*. **91**, 4470 (1987).

N.4. Force Fields

N.4.1. Force Fields from QM

197-Parameters and Validity of Force-Field Models of Silicon Using Ab Initio Calculations on Small Clusters. A. Zur, T. C. McGill, and W. A. Goddard III. In *Proceedings of the 13th International Conference on Defects in Semiconductors* (Coronado, California, August 1984); L. C. Kimerling and J. M. Parsey, Jr., Eds. (The Metallurgical Society of AIME, 1985); pp 235−241.

369-Ab Initio Derived Spectroscopic Quality Force Fields for Molecular Modeling and Dynamics. S. Dasgupta, K. A. Brameld, C.-F. Fan, and W. A. Goddard III. *Spectrochim. Acta, Part A* **53**, 1347 (1997).

281-Benzene Forms Hydrogen-Bonds with Water. S. Suzuki, P. G. Green, R. E. Bumgarner, S. Dasgupta, and W. A. Goddard III. *Science* **257**, 942 (1992).

296-Hydrogen Bonding in the Benzene−Ammonia Dimer. D. A. Rodham, S. Suzuki, R. D. Suenram, F. J. Lovas, S. Dasgupta, W. A. Goddard III, and G. A. Blake. *Nature* **362**, 735 (1993).

371-Distance Dependent Hydrogen Bond Potentials for Nucleic Acid Base Pairs for ab Initio Quantum Mechanical Calculations (LMP2/cc-pVTZ). K. Brameld, S. Dasgupta, and W. A. Goddard III. *J. Phys. Chem. B* **101**, 4851 (1997).

O. Reviews

188-The Role of Oxygen and Other Chemisorbed Species on Surface Processes for Metals and Semiconductors; Approaches to Dynamical Studies of Surface Processes. W. A. Goddard III, J. J. Low, B. D. Olafson, A. Redondo, Y. Zeiri, M. L. Steigerwald, E. A. Carter, J. N. Allison, and R. Chang. In *Proceedings of the Symposium on The Chemistry and Physics of Electrocatalysis*; J. D. E. McIntyre, M. J. Weaver, and E. B. Yeager, Eds. (The Electrochemical Society, Inc., Pennington, NJ, 1984); Vol. 84-12, pp 63−95.

193-Theoretical Chemistry Comes Alive: Full Partner with Experiment. W. A. Goddard III. *Science* **227**, 917 (1985).

200-Theoretical Chemistry Comes Alive. W. A. Goddard III. *Eng. Sci*. **49**, 2 (1985).

215-Theoretical Chemistry Comes Alive: Full Partner with Experiment. William A. Goddard III. In *Frontiers in the*

Chemical Sciences; W. Spindel and R. M. Simon, Eds. (American Association for the Advancement of Science, Washington, DC, 1986); pp 131−143.

240-Simulation of Atoms and Molecules. W. A. Goddard III. In *Biotechnology and Materials Science, Chemistry for the Future*; M. L. Good, Ed. (American Chemical Society, Washington, DC, 1988); Chapter 8, pp 71−84.

293-Atomistic Simulation of Materials. W. A. Goddard III, N. Karasawa, R. Donnelly, J. Wendel, C. B. Musgrave, J.-M. Langlois, K. T. Lim, S. Dasgupta, J. J. Gerdy, T. Maekawa, X. Chen, H.-Q. Ding, M. N. Ringnalda, R. Friesner, T. Yamasaki, T. Cagin, A. Jain, and J. Kerins. In *Molecular Modeling; The Chemistry of the 21st Century*; M. A. Chaer Nascimento, Ed. (World Scientific Publishing Co. Inc., Rio de Janeiro, Brazil, 1994).

347-Recent Developments in Quantum Mechanics and Molecular Dynamics with Applications to Problems in Materials, Catalysis, and Biochemistry. W. A. Goddard III. *Proc. 10th Inst. Fundam. Chem., 11th Symp.* (Kyoto Japan, May 1995), **57** (1996).