Jeffrey J. Gray

Department of Chemical & Biomolecular Engineering
Johns Hopkins University, 3400 N. Charles Street, Baltimore, Maryland 21218
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I. Education

The University of Texas at Austin,
Ph.D. in Chemical Engineering, August 2000

The University of Michigan, Ann Arbor
B.S.E. in Chemical Engineering, May 1994, Summa Cum Laude

II. Professional Experience

Professor, Johns Hopkins University 2014-Present
Primary Appointment: Chemical & Biomolecular Engineering

JHU Affiliations:
Faculty Member, Program in Molecular Biophysics 2002-Present
Secondary Appointment, Sidney Kimmel Comprehensive Cancer Center 2004-Present
Faculty Member, Institute for NanoBioTechnology 2006-Present

Associate Professor, Johns Hopkins University 2009-2014
Assistant Professor, Johns Hopkins University 2002-2009

Visiting Professor, University of Texas at Austin Spring 2013

Post-Doctoral Research Fellow, University of Washington 2000-2002
Advisor: David Baker
Research topic: Protein-Protein Docking

Graduate Research Assistant, The University of Texas at Austin 1994-2000
Advisor: Roger T. Bonnecaze
Thesis topic: Structure Formation in Colloidal and Nanoscale Systems

III. Selected Honors and Awards

Major honors and awards:
AIChE Himmelblau Award for Innovations in Computer-Based Chemical Engineering Education, 2016
College of Fellows, American Institute for Medical and Biological Engineering (AIMBE), 2016
Centennial Lecturer, McKetta Department of Chemical Engineering, UT-Austin, 2015
AIChE ComSEF Plenary Lecturer, 2015
F. Stuart Hodgson Faculty Scholar, 2011-2014
NSF CAREER Award, 2009
JHU Alumni Association Excellence in Teaching Award, 2006
Beckman Young Investigator Award, 2005
NIH K01 Mentored Quantitative Research Fellowship in Genomics, 2001-2006

Selected awards prior to JHU:
Celanese Outstanding Teaching Assistant Award, 1999
UT-Austin College of Engineering Teaching Excellence Award, 1999
NSF Graduate Fellowship, 1994-1997

James B. Angell Scholar, U-Michigan
Phi Beta Kappa, 1993
Tau Beta Pi, 1991

IV. Significant Awards Granted to Students Advised by J. Gray

Postdoctoral Trainees:

RosettaCon Best Talk Award, J. Labonte, 2015
Rosetta Service Award, J. Labonte, 2015
NIH F32 Post-doctoral Fellowship, J. Labonte, 2014

Graduate Students:

Hertz Foundation Fellowship, R. Alford 2016
NSF Graduate Research Fellowship, R. Alford 2016
NSF Graduate Research Fellowship, E. Lagesse, 2015
RosettaCon Best Poster Award, B. Weitzner, 2015
Rosetta Service Award, E. Lagesse, 2015
Rosetta Service Award, B. Weitzner, 2013
NIH Ruth L. Kirschstein Graduate Fellowship, M. Berrondo, 2007-2010
Genentech Second Place Poster Award, 1st International Conference on Biomolecular Engineering, D. Masica, 2007
ARCS Fellowship, M. Daily, 2004-2005

Undergraduate Students Awarded Graduate Fellowships:

(As mentioned above) Hertz Foundation and NSF Graduate Research Fellowships (to attend JHU ChemBE), R. Alford 2016
DAAD Fellowship (for graduate study at Munich), J. R. Porter, 2012
NSF Graduate Research Fellowship (to attend MIT Chemical Engineering), M.-Y. Lee, 2012
NSF Graduate Research Fellowship (to attend MIT Bioengineering), S. Schrier, 2011
NSF Graduate Research Fellowship (to attend Oxford), R. Harrison 2010
NSF Graduate Research Fellowship (to attend UCSD Biology), E. Specht 2009

Other Undergraduate Student Awards:

Monteverde Award, Mellon College of Science, R. Alford 2016
JHU Center for Educational Resources Tech Fellowship, A. Mathews, 2013
Service to Rosetta Award, E. Baugh, 2012
Provost's Undergraduate Research Award, C. Bohrson, 2012
JHU Center for Educational Resources Tech Fellowship, B. Uranukul, 2012
Fisher Award for Undergraduate Research in Cancer, M.-Y. Lee, 2011
Provost's Undergraduate Research Award, M.-Y. Lee, 2010
Elenora Streb Muly Award for Undergraduate Research, M.-Y. Lee, 2009
Pistritto Fellowship, E. Kim, 2008
JHU Center for Educational Resources Tech Fellowship, J.D. Bagert & J. Rosenberg, 2008
Provost's Undergraduate Research Award, E. Kim, 2007
Elenora Streb Muly Award for Undergraduate Research, E. Specht & S. Schrier, 2006
Provost's Undergraduate Research Award, G. Lande, 2005

High School Students:

Intel Science Talent Search Winner, Fifth Place, R. Harrison, 2005
Office of Naval Research Science Award, R. Harrison, 2004
NAACP ACT-SO Finalist, R. Harrison, 2004
Third place in Biochemistry, International Science and Engineering Fair, Portland, T. Upadhyaya, 2004

V. Publications

Total citations (as of February 2, 2016):

Scopus: 3,299 citations, h-index: 27 (455 citations in 2015)
Google Scholar: 4,524 citations, h-index: 32 (2,923 citations since 2011)

Links to Scopus and Google Scholar citation summaries at *http://graylab.jhu.edu/members.html*
Undergraduate student authors underlined.

Manuscripts in review

83. Marze N, Jeliazkov JR, Roy Burman SS, Boyken SE & **Gray JJ**, "Modeling oblong proteins and water-mediated interfaces with RosettaDock in CAPRI rounds 28-35," *Proteins* (invited)

82. Mathew MP[*], Tan E[*], Labonte JW[*], Shah S., Saeui CT, Liu L, Bhattacharya R, Bovonratwet P, **Gray JJ** & Yarema K, "Glycoengineering of esterase activity through metabolic flux-based modulation of sialic acid." ([*]Equal contribution authors)

81. Koehler Leman J, D'Avino A & **Gray JJ** 2016 "Comparison of NMR and crystal structures of membrane proteins and computational refinement to improve model quality."

80. Weitzner BD, Jeliazkov JR, Lyskov S, Marze N, Kuroda D, Frick R, Biswas N & **Gray JJ** 2016 "Modeling and docking antibody structures with Rosetta" (protocol).

79. Weitzner BD & **Gray JJ** 2016 "Accurate structure prediction of CDR H3 loops enabled by a novel structure-based C-terminal constraint."

78. Jiang, W., Pacella, M. S., Athanasiadou, D., Nelea, V., Vali, H., Hazen, R. M., **Gray, J. J.** & McKee, M. D. 2016 "Chiral amino acids induce hierarchical structure in calcium carbonate," in revision.

Papers in press

77. Kuroda, D. & **Gray, J. J.**, 2016 "Pushing the backbone in protein-protein docking," *Structure*, in press.

Peer-reviewed published works

76. Marze, N. A. & **Gray, J. J.**, 2016 "Improved Prediction of Antibody V_L-V_H Orientation," *Protein Eng. Des. Sel.*, available in Advance Access.

75. Kuroda, D. & **Gray, J. J.**, 2016 "Shape complementarity of hydrogen bond preferences in protein-protein interfaces: Implications for antibody modeling and protein-protein docking," *Bioinformatics,* available in **Advance Access**. DOI: 10.1002/prot.25007.

74. DeKosky, B. J.,* Lungu, O.I.,* Park, D., Johnson, E. L., Charab, W., Chrysostomou, C., Kuroda, D., Ellington, A. D., Ippolito, G. C., **Gray, J. J.**, & Georgiou, G. 2016 "Large-Scale Sequence and Structural Comparisons of Human Naive and Antigen-Experienced Antibody Repertoires," *Proc. Natl. Acad. Sci. U S A* **113**(19), E2636-45, PMCID: PMC4868480.

73. Lensink, M., Velankar, S., Kryshtafovych, A., Huang, S., Duhovny-Schneidman, D., Sali, A., … Marze, N., Roy Burman, S., Kuroda, D., **Gray, J. J.**, … and Wodak, S. [82 authors total] 2016 "Prediction of homoprotein and heteroprotein complexes by protein docking and template-based modeling: A CASP-CAPRI experiment," *Proteins* **Early View**.

72. Pierre, B., Labonte, J. W., Xiong, T., Aoraha, E., Williams, A., Shah, V., Chau, E., Helal, K. Y., **Gray, J. J.** & Kim, J. R. 2015 "Molecular determinants for protein stabilization by insertional fusion to a thermophilic host protein," *ChemBioChem* **16**(16), 2392-2402.

71. Matlahov, I., Iline-Vul, T., Abaiev, M., Lee, E. M.-Y., Nadav-Tsubery, M., Keinan-Adamsky, K., **Gray, J. J.** & Goobes, G. 2015 "Interfacial mineral-peptide properties of a mineral binding peptide from osteonectin and bone-like apatite," *Chem. Mater*. **27**(16), 5562-5569.

70. Alford, R. F.[*], Koehler Leman, J.[*], Weitzner, B. D., Duran, A. M., Tilley, D. C., Elazar, A. & **Gray, J. J.** 2015 "An integrated framework advancing membrane protein modeling and design," *PLoS Comput. Biol.* **11**(9): e1004398. ([*]Equal contribution authors)

69. Jiang, Q., Arnold, S., Heanue, T., Kilambi, K. P., Doan, B., Kapoor, A., Ling, A. Y., Sosa, M. X., Guy, M., Jiang, Q., Burzynski, G., West, K., Bessling, S., Griseri, P., Amiel, J., Fernandez, R. M., Verheij, J. B. G. M., Hofstra, R. M. W., Borrego, S., Lyonnet, S., Ceccherini, I., **Gray, J. J.**, Pachnis, V., McCallion, A. S., Chakravarti, A. 2015 "Functional loss of semaphorin 3C/semaphorin 3D and epistatic interaction with Ret are critical to Hirschsprung disease liability," *Am. J. Human Genetics* **96**(4), 581-596.

68. Weitzner, B. D., Dunbrack, R., & **Gray, J. J.** 2015 "The origin of CDR H3 structural diversity," *Structure* **23**(2), 302-311.

67. Koehler Leman, J., Ulmschneider, M., & **Gray, J. J.** 2015 "Computational modeling of membrane proteins," *Proteins* **83**(1), 1-24.

66. Kilambi, K. P., Reddy, K., & **Gray, J. J.** 2014 "Protein-protein docking with dynamic residue protonation states," *PLoS Comput. Biol.* **10**(12): e1004018.

65. Weitzner, B.[*], Kuroda, D.[*], Marze, N., Xu, J. & **Gray, J. J.** 2014 "Blind prediction performance of RosettaAntibody 3.0: grafting, relaxation, kinematic loop modeling, and full CDR optimization," *Proteins* **82**(8), 1611-1623.

64. Firnberg, E., Labonte, J. W., **Gray, J. J.** & Ostermeier, M. 2014 "A Comprehensive, High-Resolution Map of a Gene's Fitness Landscape," *Mol. Biol. Evol*. **31**(6), 1581-1592.

63. Lensink, M. F., all CAPRI participants (including Xu, J., Muthu, P., Kilambi, K. P., and **Gray, J. J.**), Wojdyla, J. A., Kleanthous, C., and Wodak, S. J. (56 total authors) 2014 "Blind Prediction of Interfacial Water Positions in CAPRI," *Proteins* **82**(4), 620-632.

62. Xu, J.[*], Tack, D.[*], Hughes, R. A., Ellington, A. D.[†], & **Gray, J. J.**[†] 2014 "Structure-based Non-canonical Amino Acid Design to Covalently Crosslink an Antibody-Antigen Complex," *J. Struct. Biol*. **185**(2), 215-222. ([*]Equal contribution authors; [†]co-corresponding authors; Invited contribution)

61. Kilambi, K. P., Pacella, M. S., Xu, J., Labonte, J., Porter, J., Muthu, P., Drew, K., Kuroda, D., Schueler-Furman, O., Bonneau, R., & **Gray, J. J.** 2013 "Extending RosettaDock with water, sugar, and pH for prediction of complex structures and affinities for CAPRI rounds 20-27," *Proteins* **81**(12), 2201-22019. (**Featured cover illustration**)

60. Pacella, M. S., Koo, D. C. E., Thottungal, R. A., & **Gray, J. J.** 2013 "Using the RosettaSurface Algorithm to Predict Protein Structure at Mineral Surfaces," *Method Enzymol.* **532**, 343-366.

59. Moretti, R., Fleishman, S. J., Agius, R., Torchala, M., Bates, P.A., … Pacella, M., Kilambi, K. P., **Gray, J. J.**, … Velankar, S., Janin, J., Wodak, S. J., and Baker, D. (about 70 total authors) 2013 "Community-wide Evaluation of Methods for Predicting the Effect of Mutations on Protein-Protein Interactions," *Proteins* **81**(11), 1980-1987.

58. Drew, K., Renfrew, P. D., Craven, T., Butterfoss, G. L., Chou, F.-C., Lyskov, S., Bullock, B. N., Watkins, A., Labonte, J. W., Pacella, M., Kilambi, K. P., Leaver-Fay, A., Kuhlman, B., **Gray, J. J.**, Bradley, P., Kirshenbaum, K., Arora, P. S., Das, R., & Bonneau, R. 2013 "Adding Diverse Noncanonical Backbones to Rosetta: Enabling Peptidomimetic Design," *PLoS One* **8**(7): e67051.

57. Der, B. S., Kluwe, C., Miklos, A. E., Jacak, R., Lyskov, S., **Gray, J. J.**, Georgiou, G., Ellington, A. D. & Kuhlman, B. 2013 "Alternative computational protocols for supercharging protein surfaces for reversible unfolding and retention of stability," *PLoS One* **8**(5): e64363.

56. Lyskov, S.[*], Chou F.-C.[*], Conchúir, S. Ó., Der, B. S., Drew, K., Kuroda, D., Xu, J., Renfrew, P. D., Sripakdeevong, P., Borgo, B., Havranek, J. J., Kuhlman, B., Kortemme, T., Bonneau, R., **Gray, J. J.**[†], Das, R.[†] 2013 "Serverification of Molecular Modeling Applications: the Rosetta Online Server that Includes Everyone (ROSIE)," *PLoS One* **8**(5): e63906. ([*]These authors contributed equally to this work; [†]co-corresponding authors)

55. Leaver-Fay, A., O'Meara, M., J., Tyka, M., Jacak, R., Song, Y., Kellogg, E. H., Thompson, J., Davis, I. W., Pache, R. A., Lyskov, S., **Gray, J. J.**, Kortemme, T., Richardson, J. S., Havranek, J. J., Snoeyink, J., Baker, D. & Kuhlman, B., 2013 "Scientific Benchmarks for Guiding Macromolecular Energy Function Improvement," *Method Enzymol.* **523**, 109-143.

54. Tarasevich, B. J., Perez-Salas, U. Masica, D. L., Philo, J., Kienzle, P., Srueger, S., Majkrzak, C. F., **Gray, J. J.**, & Shaw, W. J., 2013 "Neutron Reflectometry Studies of the Adsorbed Structure of the Amelogenin, LRAP," *J. Phys. Chem. B* **117**(11), 3098-3109.

53. Chaikind, B., Kilambi, K. P., **Gray, J. J.**, & Ostermeier, M., 2012 "Targeted DNA Methylation using an Artificially Bisected M.HhaI Fused to Zinc Fingers," *PLoS One* **7**(9), e44852.

52. Ye, Y., Stahley, M. R., McKnight, J. N., Friedman, J. I., Xu, J., Sun, Y., **Gray, J. J.**, Bowman, G. D. & Stivers, J. T. 2012 "Enzymatic Excision of Uracil Residues in Nucleosomes Depends on Local DNA Structure and Dynamics," *Biochemistry* **51**(30), 6028-6038.

51. Kilambi, K.P. & **Gray, J. J.** 2012 "Rapid Calculation of Protein pK_a Values using Rosetta," *Biophys. J*. **103**(3), 587-595.

50. Miklos, A. E., Kluwe, C., Der, B. S., Pai, S., Sircar, A., Hughes, R. A., Berrondo, M., Xu, J., Codrea, V., Buckley, P. E., Calm, A. M., Welsh, H. S., Warner, C. R., Zacharko, M. A., Carney, J. P., **Gray, J. J.**, Georgiou, G., Kuhlman, B., & Ellington, A. D. 2012 "Structure-Based Design of Supercharged, Highly Thermoresistant Antibodies," *Chemistry & Biology* **19**(4), 449-455.

49. Schrier, S. B., Sayeg, M. K., & **Gray, J. J.** 2011 "Prediction of Calcite Morphology from Computational and Experimental Studies of Mutations of a De Novo Designed Peptide," *Langmuir* **27**(18), 11520-11527.

48. Fleishman, S. J., Whitehead, T. A., Strauch, E. M., and about 95 others including **Gray, J. J.**, Kilambi, K. P., and Sircar, A., 2011 "Community-Wide Assessment of protein-Interface Modeling Suggests Improvements to Design Methodology," *J. Mol. Biol.* **414**(2), 289-302.

47. Baugh, E., Lyskov, S., Weitzner, B. D., & **Gray, J. J.** 2011 "Real-time PyMOL visualization for Rosetta and PyRosetta," *PLoS One*, **6**(8): e21931.

46. Chaudhury, S., Berrondo, M., Weitzner, B. D., Muthu, P., Bergman, H., & **Gray, J. J.** 2011 "Benchmarking and analysis of protein docking performance in RosettaDock 3.2," *PLoS One* **6**(8): e22477.

45. Berrondo, M., **Gray, J. J.** 2011 “Computed structures of point deletion mutants and their enzymatic activities,” *Proteins* **79**(10), 2844-2860. (**Featured cover illustration**)

44. Masica, D. L., **Gray, J. J.**†, & Shaw, W.† 2011 “Partial high-resolution structure of phosphorylated and non-phosphorylated leucine-rich amelogenin protein adsorbed to hydroxyapatite,” *J. Phys. Chem. C*. **115**(28), 13775-13785. (†co-corresponding authors)

43. Sircar, A., Sanni, K., Shi, J., & **Gray, J. J.** 2011 “Analysis and Modeling of the Variable Region of Camelid Single Domain Antibodies,” *J. Immunology* **186**(11), 6357-6367.

42. McKee, M. D., Nakano, Y., Masica, D. L., **Gray, J. J.**, Lemire, I., Heft, R., Crine, P., & Millan J. L., 2011 “Enzyme Repleacement Therapy Prevents Dental Defects in a Model of Hypophosphatasia,” *J. Dental Res.* **90**(4), 470-476. (**Featured cover illustration**)

41. Bocik, W. E., Sircar, A., **Gray, J. J.**†, & Tolman, J. R.† 2011 “Mechanism of polyubiquitin chain recognition by the human ubiquitin conjugating enzyme Ube2g2,” *J. Biol. Chem.* **286**, 3981-3991. (†co-corresponding authors)

40. Leaver-Fay, A., Tyka, M., Lewis, S.M., Lange, O.F., Thompson, J., Jacak, R., Kaufman, K., Renfrew, P.D., Smith, C.A., Sheffler, W., Davis, I.W., Cooper, S., Treuille, A., Mandell, D.J., Fichter, F., Ban, Y.-E.A., Fleishman, S.J., Corn, J.E., Kim, D.E., Lyskov, S., Berrondo, M., Mentzer, S., Popovic, Z., Havranek, J.J., Karanicolas, J., Das, R., Meiler, J., Kortemme, T., **Gray, J. J.**, Kuhlman, B., Baker, D., Bradley, P., 2011 “Rosetta3: An object-oriented software suite for the simulation and design of macromolecules,” *Method Enzymol.* **487**, 545-574.

39. Masica, D. L., Ashworth, J., Ndao, M., Drobny, G., **Gray, J. J.**, 2010 “Toward a structure determination method for biomineral-associated protein using combined solid-state NMR and computational structure prediction,” *Structure,* **18**(12), 1678-1687.

38. Keshet, B., **Gray J. J.**, & Good, T. A. 2010 “Structurally Distinct Toxicity Inhibitors Bind at Common Loci on β-Amyloid Fibril,” *Protein Science* **19**(12), 2291-2304.

37. Sircar, A., Chaudhury, S., Kilambi, K.P., Berrondo, M., & **Gray, J. J.** 2010 “A generalized approach to sampling backbone conformations with RosettaDock for CAPRI rounds 13-19,” *Proteins* **78**(15), 3115-3123.

36. Masica, D. L., Schrier, S. B., Specht, E., **Gray J. J.**, 2010 “De novo design of peptide-calcite biomineralization systems,” *J. Am. Chem. Soc.* **132**(35), 12252-12262.

35. Berrondo, M., **Gray, J. J.**, & Schleif, R., 2010 “Computational predictions of the mutant behavior of AraC,” *J. Mol. Biol.* **298**(3), 462-470.

34. Addison, W. N., Masica, D. L., **Gray, J. J.**, & McKee, M. D., 2010 “Phosphorylation-dependent inhibition of mineralization by osteopontin ASARM peptides is regulated by PHEX cleavage,” *J. Bone & Mineral Res.* **25**(4), 695-705.

33. Chaudhury, S., Lyskov, S., **Gray, J. J.**, 2010 “PyRosetta: a script-based interface for implementing molecular modeling algorithms using Rosetta,” *Bioinformatics* **26**(5), 689-691.

32. Sircar, A., **Gray, J. J.**, 2010 “SnugDock: Paratope structural optimization during antibody-antigen docking compensates for errors in antibody homology models,” *PLoS Comput. Biol.* **6**(1): e1000644.

31. Chaudhury, S. & **Gray, J. J.**, 2009 “Identification of structural mechanisms of HIV-1 protease specificity using computational peptide docking and implications for drug resistance,” *Structure* **17**(12), 1636-1648.

30. Chien, Y.-C., Masica, D.L., **Gray, J. J.**, Nguyen, S., Vali, H., & McKee, M. D. 2009 "Modulation of calcium oxalate dehydrate growth by selective crystal-face binding of phosphorylated osteopontin and poly-aspartate peptide showing occlusion by sectoral (compositional) zoning," *J. Biol. Chem.* **284**, 23491-23501.

29. Sircar,[*] A., Kim,[*] E.T., & **Gray, J. J.** 2009 "RosettaAntibody: Antibody Variable Region Homology Modeling Server," *Nucleic Acids Res.* **37** (Web Server Issue), W474-W479. ([*]These authors contributed equally to this work)

28. Masica, D. L. & **Gray, J. J.** 2009 "Solution- and adsorbed-state structural ensembles predicted for the statherin-hydroxyapatite system," *Biophys. J.* **96**(8), 3082-3091.

27. Daily, M. D. & **Gray, J. J.** 2009 "Allosteric communication occurs via networks of tertiary and quaternary motions in proteins," *PLoS Comput. Biol*. **5**(2), e1000293.

26. Sivasubramanian, A., Sircar, A. & **Gray, J. J.** 2009 "Toward high-resolution homology modeling of antibody F_v regions and application to antibody-antigen docking," *Proteins* **74**(2), 497-514.

25. Chaudhury, S. & **Gray, J. J.** 2008 "Conformer selection and induced fit in flexible backbone protein-protein docking using computational and NMR ensembles," *J. Mol. Biol.* **381**(4), 1068-1087.

24. Lyskov, S. & **Gray, J. J.**, 2008 "The RosettaDock server for local protein-protein docking," *Nucleic Acids Res.* **36** (Web Server Issue), W233-W238.

23. Pickin, K., Chaudhury, S., Dancy, B., **Gray, J. J.**, & Cole, P. 2008 "Analysis of protein kinase autophosphorylation using expressed protein ligation and computational modeling," *J. Am. Chem. Soc.* **130**(17), 5667-5669.

22. Berrondo, M., Ostermeier, M. & **Gray, J. J.** 2008 "Structure prediction of domain insert proteins from structures of individual domains," *Structure* **16**(4), 513-527.

21. Daily, M. D., Upadhyaya, T. & **Gray, J. J.** 2008 "Contact rearrangements form coupled networks from local motions in allosteric proteins," *Proteins* **71**(1), 455-466.

20. Sivasubramanian, A., Maynard, J. A. & **Gray, J. J.** 2008 "Modeling the structure of mAb 14B7 bound to the anthrax protective antigen," *Proteins* **70**(1), 218-230.

19. Makrodimitris, K., Masica, D. L., Kim, E. T. & **Gray, J. J.** 2007 "Structure prediction of protein-solid surface interactions reveals a molecular recognition motif of statherin for hydroxyapatite," *J. Am. Chem. Soc*. **129**(44), 13713-13722.

18. Chaudhury,[*] S., Sircar,[*] A., Sivasubramanian, A., Berrondo, M. & **Gray, J. J.** 2007 "Incorporating biochemical information and backbone flexibility in RosettaDock for CAPRI rounds 6-12," *Proteins* **62**(4), 792-800. ([*]These authors contributed equally to this work.)

17. Meitzler, J. L., **Gray, J. J.** & Hendrickson, T. L. 2007 "Truncation of the caspase-like subunit (Gpi8p) of *Saccharomyces cerevisiae* GPI transamidase: Dimerization revealed," *Arch. Biochem. Biophys.* **462**(1), 83-93.

16. Daily, M. D. & **Gray, J. J.** 2007 "Local motions in a benchmark of allosteric proteins," *Proteins* **67**(2), 385-399. (**Featured cover illustration**)

15. **Gray, J. J.** Fall 2006 "Biomolecular modeling in a chemical engineering process dynamics and control course," *Chem. Eng. Ed*. **40**(4), 297-306.

14. **Gray, J. J.** 2006 “High-resolution protein-protein docking,” *Curr. Opin. Struct. Biol.* **16**(2), 183-193.

13. Sivasubramanian, A., Chao, G., Pressler, H. M., Wittrup, K. D., & **Gray, J. J.** 2006 “Structural model of the mAb 806-EGFR complex by computational docking followed by computational and experimental mutagenesis,” *Structure* **14**(3), 401-414.

12. Daily, M. D., Masica, D., Sivasubramanian, A., Somarouthu, S., & **Gray, J. J.** 2005 “CAPRI Rounds 3-5 Reveal Promising Successes and Future Challenges For RosettaDock,” *Proteins* **60**(2), 181-186. (**Featured cover illustration**)

11. Singh, P., Mhaka, A. M., Christensen, S. B., **Gray, J. J.**, Denmeade, S. R., & Isaacs, J. T. 2005 “Applying Linear Interaction Energy Method for Rational Design of Non-Competitive Allosteric Inhibitors of the SERCA ATPase,” *J. Med. Chem.* **48**(8), 3005-3014.

10. **Gray, J. J.** 2004 “The Interaction of Proteins with Solid Surfaces,” *Curr. Opin. Struct. Biol.* **14**(1), 110-115.

9. **Gray, J. J.**, S. E. Moughan, C. Wang, O. Schueler-Furman, B. Kuhlman, C.A. Rohl, D. Baker. 2003 “Protein-Protein Docking with Simultaneous Optimization of Rigid Body Displacement and Side Chain Conformations,” *J. Mol. Biol.* **331**(1), 281-299.

8. **Gray, J. J.**, S. E. Moughan, T. Kortemme, O. Schueler-Furman, K.M.S. Misura, A.V. Morozov, D. Baker. 2003 “Protein-Protein Docking Predictions for the CAPRI Experiment,” *Proteins* **52**(1), 118-122.

7. **Gray, J. J.** & Bonnecaze, R. T. 2001 “Adsorption of Charge-Bidisperse Mixtures of Colloidal Particles,” *Langmuir,***17**(25), 7935-7947.

6. **Gray, J. J.**, Klein, D. H., Korgel, B. A. & Bonnecaze, R. T. 2001 “Microstructure Formation and Kinetics in the Random Sequential Adsorption of Polydisperse Tethered Nanoparticles Modeled as Hard Disks,” *Langmuir*, **17**(8), 2317-2328.

5. **Gray, J. J.** & Bonnecaze, R. T. 2001 “Adsorption of Colloidal Particles by Brownian Dynamics Simulation: Kinetics and Surface Structures,” *J. Chem. Phys.,* **114**(3), 1366-1381.

4. **Gray, J. J.**, Klein, D. H., Bonnecaze, R. T. & Korgel, B. A. 2000 “Non-Equilibrium Phase Behavior During the Random Sequential Adsorption of Tethered Hard Disks,” *Phys. Rev. Lett.,* **85**(21), 4430-4433.

3. **Gray, J. J.**, Chiang, B. & Bonnecaze, R. T. 1999 “Origin of Anomalous Multibody Interactions,” *Nature*, **402**, 750 (brief communication).

2. **Gray, J. J.** & Bonnecaze, R. T. 1998 “Rheology and Dynamics of Sheared Arrays of Colloidal Particles,” *J. Rheology*, **42**(5), 1121-1151.

1. Lee, G. M., **Gray, J. J.** & Palsson, B. Ø. 1991 “Effect of Trisodium Citrate Treatment on Hybridoma Cell Viability,” *Biotechnol. Techniques*, **5**(4), 295-298. [*Biotechnol. Techniques* is now merged with *Biotechnol. Lett.,*

Published proceedings

1. Matsumoto, E., Tumer, I. Y., Arthur, L. F., **Gray, J. J.**, Vogler, T., Jaramillo, N., & Barr, R. 1997 “Establishing an ASEE Student Chapter: Issues for Graduate Students,” *ASEE National Conference* (proceedings), Milwaukee, WI, June 1997.

Books

1. **Gray, J. J.**, Chaudhury, S., Lyskov, S. & Labonte, J. W., *The PyRosetta Interactive Platform for Protein Structure Prediction and Design: A Set of Educational Modules*, Baltimore:CreateSpace, Second edition, 2013. (First edition: Lulu.com, 2009).

Book Chapters

1. Roehrich, A., Ash, J., Zane, A., Masica, D. L., **Gray, J. J.**, Goobes, G. & Drobny, G., "Solid-State NMR Studies of Biomineralization Peptides and Proteins," in *Proteins at Interfaces III: State of the Art*, Ed. Horbett, T., Brash, J. L. & Norde, W., American Chemical Society, Oxford University Press, 2013.

VI. Research Support (Gray is PI unless noted)

Total: Approximately **$7.3 Million** to the Gray research group (2002-2016)

Current research support

1. NIH 5R01-GM078221, "Prediction of the structure of therapeutic antibodies with their antigens," 9/1/2012-8/31/2016, $1,241,054 ($821,600 direct).
   Administrative supplement: $48,753 for training of Rebecca Alford, 11/1/2013-10/31/2015.

2. NSF/DMR 1507736, "Directed Biomineralization: Designing Peptides to Control Crystal Nucleation and Growth," 8/1/2015-7/31/2018, $360,000.

3. NIH 2R01-GM73151, "Rosetta: An Integrated Protein Structure Modeling Suite," (PI: Brian Kuhlman, UNC), 9/1/2013-4/30/2017, $618,000 total / $416,000 direct to Gray lab.

4. NSF/DBI 1541278, "EAGER: A New Model for Undergraduate Training: A Virtual Community of Researchers in Computational Biomolecular Structure and Design," 5/1/2015-4/30/2017, $207,669.

5. DTRA CB3636, "Ruggedized Antibody Program," (PI: Alex Miklos, Edgewood Chemical Biological Center), 9/1/2014-8/31/2016, $200,000 subcontract to Gray lab.

6. Rosetta Licensing Fund, "Rosetta Testing Services," 7/1/2014-6/30/2015, $50,000 direct to Gray lab.

Pending research support

7. NIH R01-GM078221 competitive renewal, "Prediction of the structure of therapeutic antibodies with their antigens," 4/1/2017-3/30/2022, $1,250,000 direct.

8. NIH/PPG "Biochemical Mechanisms of Phosphatidylinositol (3,4,5)-trisphosphate (PP3) regulation," 12/1/2016-11/30/2021, $8,095,398 (Gray is co-PI of the Computational Core, 1 month).

Completed research support

1. NSF/CBET 0846324, "CAREER: Structure Prediction of Proteins on Solid Surfaces," 3/1/2009-2/28/2015, $400,000 ($250,000 direct).

2. Rosetta Licensing Fund, “Object-Oriented Framework for Membrane Protein Modeling,” 12/1/2014-11/30/2015, $20,000 direct to Gray lab.

3. NIH U54-RR020839, “Networks, Pathways and Dynamics of Lysine Modification,” (PI: Jef D. Boeke, JHU), 8/1/2009-7/31/2014, ~$40,000 to Gray lab.

4. NIH R01-GM73151, “Rosetta: An Integrated Protein Structure Modeling Suite,” (PI: Brian Kuhlman, UNC), 3/1/2005-2/28/2009, $201,678 to Gray lab ($123,619 direct); 9/1/2009-8/31/2013, $598,400 to Gray lab (~$370,000 direct).

5. NSF/MCB 0919377, “Structure-function studies of the allosteric mechanisms of protein switches,” (PI: Marc Ostermeier), 2009-2013, $654,924 ($418,500 direct; ~1/3 to Gray lab).

6. NIH R01-DE015347, “Solid state NMR structure/function studies of amelogenin,” 7/1/2010-6/30/2013 (PI: Wendy Shaw, Pacific Northwest National Lab). $75,000 to Gray lab.

7. DARPA, “Unnatural amino acid augmentation of computational antibody design (UnACAD),” 3/15/2010-12/14/2012 (PI: George Georgiou, UTexas). $595,384 to Gray lab ($381,400 direct).

8. NIH R01-GM078221, “Prediction of the structure of therapeutic antibodies with their antigens,” 9/1/2006-8/31/2012, $1,362,812 ($871,250 direct).

9. UCB Celltech Corporation Research Contract, “Combined structure prediction and NMR approach toward antibody structure determination and docking,” 3/1/2008-2/28/2011, $269,581 ($183,581 direct).

10. Beckman Young Investigator Award, “Design of Specific Protein Interactions with Solid Surfaces,” 9/1/2005-8/31/2009, $264,000 direct.

11. Chemical Therapeutics Working Group, Sidney Kimmel Comprehensive Cancer Center, “Preliminary structural models of the anti-cancer monoclonal antibody 806 binding to the epidermal growth factor receptor,” 2005, $25,000 direct.

12. NIH K01-HG002316, “Computational Prediction of Protein-Protein Docking for Genomic Analysis,” 6/22/2001-8/31/2006, $569,364 ($529,930 direct).

13. American Chemical Society Petroleum Research Fund, “Structure of Rigid and Unfolding Proteins on Solid Surfaces,” 2004-2006, $35,000 direct.

Equipment support

1. IBM BladeCenter computing cluster with 60 CPUs, purchased through Whiting School Bloomberg funds matched by IBM, 2003, total value $167,000.

2. Gigatrend 0.5 TB server and backup system, $5,966 donation matched by Whiting School Bloomberg funds toward equipment with a total value of $20,328, 2004.

3. Dell quad-core computing cluster with 140 CPUs, $57,490 donation matched by Whiting School Bloomberg funds towards equipment with a total value of $146,000, 2006.

Current computational support

1. XSEDE / Texas Advanced Computing Center, TG-MCB130172, "Stampede Power for the ROSIE Gateway," 2013-2014, 331,102 service units and extended computing support services; 2014-2015, 433,583 service units (SU, roughly CPU-h) and extended computing support services; 2015-2016, 661,729 SU (valued at $22,905)

2. XSEDE / Texas Advanced Computing Center, TG-MCB130184, "Antibody Structural Modeling and Docking," 2013-2014, 660,888 SU; 2014-2015, 379,509 SU; 2015-2016, 866,020 SU (valued at $29,983).

Completed computational support

3. TeraGrid / San Diego Supercomputing Center / IBM Blue Gene, TG-MCB080005, "Structure Prediction of Domain Insertion Proteins from Structures of the Individual Domains," 2008, 400,000 resource units.

4. XSEDE / Texas Advanced Computing Center, TG- MCB130133, "Gray Lab Startup," 2013, 200,000 service units and extended computing support services.

VII. Research Supervision

Postdoctoral Trainees

1. Dr. Arvind Sivasubramanian, 2004-2008, Therapeutic Antibodies.
   Currently: Scientist in Computational Biology, Adimab, Inc., San Francisco, CA
2. Dr. Kosta Makrodimitris, 2005-2007, Protein-Surface Interactions
   Currently: Global Bio Health Tech Center, Baltimore, MD
3. Dr. Rahul Bhowmik, 2007-2009, Protein-Surface Interactions
   Currently: Defense and Veterans Brain Injury Center (DoD), Rockville, MD
4. Dr. Myunggi Yi, 2010-2011, Mechanisms of Protein Molecular Switches
   Currently: Assistant Professor of Biomedical Engineering, Pukyong National University, South Korea
5. Dr. Monica Berrondo, 2010-2011, Protein-Protein Docking and Antibody Engineering
   Currently: Founder/CEO, Macromoltek Inc.
6. Dr. Jianqing Xu, 2010-2012, Antibody Prediction, Docking and Design
   Currently: MedImmune (AstraZeneca), Cambridge, UK
7. Dr. Daisuke Kuroda, 2011-2014, Antibodies and Flexible Backbone Docking
   Currently: Assistant Professor, Showa University (Tokyo)
8. Dr. Jason Labonte, 2011-present, Molecular Switches (with M. Ostermeier) and Glycoprotein Modeling (with K. Yarema) **NIH F32 Fellowship**
9. Dr. Julia Koehler, 2012-2016, Membrane Protein Modeling and Docking
10. Dr. Brian Weitzner, 2015-2016, Antibody Modeling

Ph.D. Students

1. Michael Daily, Program in Molecular Biophysics, Ph.D. 2008
   Thesis: *Systematic analysis of motions and communication networks in a benchmark of allosteric proteins*
   Currently: Research Scientist, Pacific Northwest National Lab, Richland, WA
2. David Masica, Program in Molecular Biophysics, Ph.D. 2009
   Thesis: *Structure Determination and Design of Biomineral-Associated Proteins*
   Currently: Post-doctoral research fellow with Rachel Karchin, JHU BME
3. Aroop Sircar, Chemical & Biomolecular Engineering, PhD 2010
   Thesis: *Computational Antibody Structure Prediction and Antibody-Antigen Docking*

Currently: EMD Serono, Boston, MA

4. Monica Berrondo, Chemical & Biomolecular Engineering, PhD 2010 **NIH Kirschstein Fellow**
   Thesis: *Prediction of the Structure and Function of Protein Mutants*
   (Gray was primary advisor; secondary advisor: Marc Ostermeier)
   Currently: Founder/CEO, Macromoltek Inc., Austin, TX
5. Sidhartha Chaudhury, Program in Molecular Biophysics, PhD 2010
   Thesis: *Using Computational Protein Docking to Model the Structure and Specificity of Protein Interactions*
   Currently: Biotechnology High Performance Computing Software Application Institute, Fort Detrick, MD
6. Krishna Kilambi, Chemical & Biomolecular Engineering, PhD 2015
   Thesis: *Computational Prediction of Protein-Protein Interactions*
   Currently: Postdoctoral Research Scientist, Biogen Idec, Boston
7. Brian Weitzner, Chemical & Biomolecular Engineering, PhD 2015
   Thesis: *Next-Generation Antibody Modeling*
   Currently: Postdoc Fellow in David Baker's lab, University of Washington
8. Michael Pacella, Biomedical Engineering, 2010-present
9. Nicholas Marze, Chemical & Biomolecular Engineering, 2011-present
10. Shourya Sonkar Roy Burman, Chemical & Biomolecular Engineering, 2012-present
11. Jeliazko Jeliazkov, Program in Molecular Biophysics, 2014-present
12. Elizabeth Lagesse, Chemical & Biomolecular Engineering, 2015-present **NSF GRF**
13. Rebecca Alford, Chemical & Biomolecular Engineering, 2015-present **Hertz & NSF GRF**

Secondary Advisor

14. Pratap Singh, Chemical & Biomolecular Engineering, Ph.D. 2007
    (Gray was co-advisor; primary adviser: John Isaacs, JHU Oncology)
    Currently: Research Scientist, Pfizer Inc., Chesterfield, MO
15. Rahel Frick, Biosciences/Immunology PhD Student, University of Oslo Rikshospitalet, Oslo, Norway (Visiting PhD student, 2016)

M.S. Students

1. Lian Guo (2002-2004), Chemical & Biomolecular Engineering, M.S. 2004
   Thesis: *Docking HPr to HPr Kinase with Partial Backbone Flexibility*
   Currently: IBM TJ Watson Research Center, NY.
2. Pravin Muthu, Chemical & Biomolecular Engineering B.S./M.S. 2011
   Thesis: *A comparison of sequence and structure based approaches for enzyme specificity design*
   Currently: PhD program, Emory University
3. Robin Thottungal, Program in Molecular Biophysics, M.S. 2011
4. Boon Uranukul, Chemical & Biomolecular Engineering, M.S. 2013
5. Xiaotong Zuo, Chemical & Biomolecular Engineering, 2014-present
6. Naireeta Biswas, Chemical & Biomolecular Engineering, 2015-present
7. Joseph Lubin, Chemical & Biomolecular Engineering, 2015-present
8. Xiyao Long, Chemical & Biomolecular Engineering, 2016-present

Research Staff

1. Sergey Lyskov, Software Engineer, M.S. Physics, Moscow
   Director of Testing for Rosetta, 2007-present
2. Matthew Mulqueen, Computer Systems Administrator, 2012-present

Undergraduates

1. Cameron White, Chemical & Biomolecular Engineering, 2016-present
2. Sofia Bali, New Mexico State University Biochemistry, REU summer 2016

3. Laura Beth Fulton, U-Pitt Mechanical Engineering, summer 2016
4. Daniel Kaganov, Chemistry and Computer Science, 2016-present
5. Kayvon Tabrizi, Chemical & Biomolecular Engineering, 2016-present
6. Gabriella Sinclair, Chemical & Biomolecular Engineering, 2015-present
7. Morgan Nance, UC-Davis Biochemistry and Molecular Biology, REU summer 2015
   (entered ChemBE PhD program at JHU)
8. Nikhil Shah, Chemical & Biomolecular Engineering, 2014-present
9. Andrew D'Avino, Biology, 2014-2016
   (co-author on paper #81, entered post-bac program at Broad Institute)
10. Shuoyang Eric Li, Chemical & Biomolecular Engineering, 2014
11. Sydney Solomon, Chemical & Biomolecular Engineering, 2014
12. Alex Mathews, Computer Science, 2013-2014
13. Michael Porter, Chemical & Biomolecular Engineering, 2013-2014
14. Rebecca Alford, Carnegie Mellon Chemistry & Computer Science, 2013-2016
    (co-first-author on paper #71; entered ChemBE PhD program at JHU)
15. Meera Valliath, Chemical & Biomolecular Engineering, 2013-2014
16. Nathan Kato, Chemical & Biomolecular Engineering, 2013
17. Jennifer Lu, Chemical & Biomolecular Engineering, 2013
18. Boon Uranukul, Chemical & Biomolecular Engineering, 2012-2013
    (entered ChE PhD program at MIT)
19. Emily Koo, Biophysics, 2012-2013
    (co-author on paper #61, entered PhD program at NYU)
20. Kavan Reddy, Chemical & Biomolecular Engineering, 2012-2013
21. Thuy-My Le, Chemical & Biomolecular Engineering, 2012-2013
22. Kathleen Rand, Chemical & Biomolecular Engineering, 2012-2013
23. Michael Seung, Chemical & Biomolecular Engineering, 2012-2014
24. Eric Lorenz, Chemical & Biomolecular Engineering and Applied Math, 2012
25. Craig Bohrson, Biomedical Engineering, 2011-2012
26. Evan Baugh, Chemical & Biomolecular Engineering, 2010-2011
    (first author on paper #47, entered PhD program at NYU)
27. Hannah Bergman, Chemical & Biomolecular Engineering, 2010
28. Joshua Austin, U Maryland Baltimore County Computer Eng. / Math, REU Summer 2010
29. Justin Porter, Biophysics, 2010-2012
    (co-author on paper #62, won DAAD Fellowship for graduate study at Munich)
30. Marianna Sayeg, Chemical & Biomolecular Engineering, 2009-2012
    (co-author on paper #48, entered ChE PhD program at Tufts)
31. Moon-Young (Liza) Lee, Chemical & Biomolecular Engineering and Biology, 2008-2012
    (co-author on paper #65, NSF Graduate Research Fellow, entered ChE PhD program at MIT)
32. Paul Nunley, Biology, 2009-2010
33. Nathaniel Tippens, Biomedical Engineering, 2009-2010
34. Sarah Schrier, Chemical & Biomolecular Engineering, 2006-2010
    (first author on paper #48, co-author on paper #37; NSF Graduate Research Fellow, entered PhD program MIT BioE)
35. Andy Chen, Chemical & Biomolecular Engineering, 2009 (entered MPH program at UMich)
36. Kayode Sanni, U. Maryland Baltimore County, Computer Engineering, REU Summer 2009
    (entered EE PhD program at JHU)
37. Eric Kim, Biomedical Engineering & Computer Science, 2006-2009
    (co-author on paper #19; now at D.E. Shaw Research)
38. Elizabeth Specht, Chemical & Biomolecular Engineering, 2006-2009
    (co-author on paper #37, NSF Graduate Fellow, entered PhD program, UCSD Biology)
39. Tiara Byrd, Florida A & M, Chemistry, REU Summer 2008

(entered PhD program in Translational Biology and Molecular Medicine as HHMI Scholar at Baylor College of Medicine)

40. Ryan Harrison, Biomedical Engineering, 2005-2007
    (NSF Graduate Research Fellow, entered PhD program at Oxford)
41. Jason Hortiatis, Chemical & Biomolecular Engineering, 2006-2007
42. Constantine Chrysostomou, Chemical & Biomolecular Engineering, 2006-2007
    (entered UTexas ChE PhD program)
43. Tarak Upadhyaya, MIT, Computer Science, REU 2004, 2005, 2006
    (co-author on paper #21)
44. Eleanor Glifort, Chemical & Biomolecular Engineering, 2005-2006
    (entered Drexel ChE PhD program)
45. Terence Lee, Computer Science, 2005-2006
46. Amanda Pace, Chemical & Biomolecular Engineering, 2005-2006
47. Galen Lande, Biophysics, 2004-2006
48. Kurt Pipenbrink, Biophysics, 2004-2005 (entered Notre Dame Chemistry PhD program)
49. Tony Lu, Chemical & Biomolecular Engineering, 2004
50. Katherine Peterson, Univ. of Utah, Chemical Engineering, REU 2004
51. Hsuan Lai, Biomedical Engineering, 2003

High School Students

1. Yash Bhatnagar, Thomas Jefferson High School for Science and Technology (Alexandria, VA, 12th grade), Summer 2013. *Currently*: Duke University (Engineering)
2. Damjan Nisevic, Baltimore Polytechnic Institute (12th grade), 2012-2013
3. Sunmoon Choi, Garrison Forest School (11th grade), 2010-2011.
4. Sal Ndao, Baltimore Polytechnic Institute (10th grade) and the Baltimore Ingenuity project, Spring 2006
   Placement: Stanford Engineering
5. Ryan Harrison, Baltimore Polytechnic Institute and the Ingenuity Project, 2003-2005
   Currently: Graduate student at Oxford/NIH with an NSF Graduate Fellowship

Lab Visitors

1. Prof. Eric Fernandez, University of Virginia Chemical Engineering, Sabbatical 2006
2. Rahel Frick, PhD student, University of Oslo, Spring 2016

VIII. Invited Seminars and Talks

2016

76. "Best Practices in Collaborative Software Development: Lessons Learned in the Rosetta Commons," *American Institute of Chemical Engineers Annual Meeting*, San Francisco, CA, November 2016.

75. "Structural modeling of antibodies and antibody-antigen complexes," *Immunotherapy 2016*, Havana, Cuba, October 2016.

74. "Structural Modeling of Glycoproteins and Protein-Sugar Complexes," National Institute of Standards and Technology (NIST), Gaithersburg, MD, 20 June 2016.

73. "Accurate global docking in RosettaDock is masked by difficult multi-domain targets in CAPRI rounds 31–35," *6th CAPRI Evaluation Meeting*, Tel Aviv, Israel, 17 April 2016.

72. "Computational Protein Engineering of Crystal Growth, Membrane Proteins, and Glycoproteins," University of Delaware Center for Biomanufacturing Science and Technology, 23 March 2016.

2015

71. "Proteins Dancing the Texas Two-Step," Centennial Lecture Series, McKetta Department of Chemical Engineering, University of Texas at Austin, 1 December 2015.

70. "Toward Structure Prediction and Design of Protein Glycosylations," Computational Science and Engineering Forum (ComSEF) Plenary Lecture, *American Institute of Chemical Engineers Annual Meeting*, Salt Lake City, November 2015.

69. "How Proteins Dance with their Partners," Inaugural Professorial Lecture, Whiting School of Engineering, Johns Hopkins University, 24 September 2015.

68. "Design and Structure Prediction of Proteins that Control Biomineralization," Technische Universität Dresden, "From Biomineralization to Materials Science" Seminar Series, 12 June 2015.

2014

67. "Computational Design of Peptides to Control Calcite Growth," *Gordon Research Conference on Biomineralization*, New London, NH, 20 August 2014.

66. "Diversity Efforts within the Rosetta Commons," *Rosetta Developers Conference*, Leavenworth, WA, 1 August 2014.

65. "Applying Rosetta to Antibody Loop Modeling and Docking," *16th Annual Phage and Yeast Display of Antibodies and Recombinant Proteins Conference*, Cambridge Healthtech Institute Protein Engineering Summit (PEGS), Boston, May 6, 2014.

2013

64. "Antibody Homology Modeling, Docking, and Design," *IBC Antibody Engineering and Therapeutics*, Long Beach, CA, 8 December 2013 (delivered by graduate student Brian Weitzner during Gray's paternity leave).

63. "Expanding RosettaDock with water and sugar and pH for predictions of complex structures and affinities," *5th CAPRI Evaluation Meeting*, Utrecht, The Netherlands, 19 April 2013.

62. "Design and Prediction of Proteins that Control Biomineralization," Chemical and Biomolecular Engineering Seminar, *Rice University*, Houston, Texas, 31 January 2013.

2012

61. "Motion and Communication Networks in Allosteric Proteins," Bioengineering Seminar, *University of Maryland College Park*, College Park, Maryland, 9 November 2012.

60. "Computational Analysis of HIV: Protein Structure, Specificity, and Drug Resistance," *Institute for Computational Medicine and Institute for Clinical and Translational Research Symposium on Computational Medicine*, Johns Hopkins Medical Institute, Baltimore, MD, 24 September 2012.

59. "Protein Docking Methods and Applications," *Hebrew University*, Jerusalem, Israel, 23 May 2012.

58. "Computational Structure Prediction and Design of Biomineralization Proteins," *Bar-Ilan University*, Ramat-Gan, Israel, 21 May 2012.

57. “Toward a Computational Pipeline from Antibody Homology Modeling to Docking to Design,” *ACS Annual Meeting*, Computer Aided Drug Design Symposium, San Diego, 26 March 2012

2011

56. “Structure Prediction of Fv and VHH Domains and Docking to their Antigens,” *Antibody Engineering and Antibody Therapeutics*, San Diego, 5 December 2011.

55. “Design and Prediction of the Behavior of Proteins on Solid Surfaces,” *Institute for Biophysical Research Retreat*, Baltimore, MD, September 2011.

54. “Design of Peptide-Biomineral Interactions using Protein Structure Prediction Methods,” *Pro-Surf: Modeling Protein Interactions with Solid Surfaces and Nanoparticles*, CECAM workshop, Lausanne, Switzerland, 9-11 May 2011.

53. “Biomolecular Engineering via Protein Structure Prediction Methods,” Chemical & Biological Engineering Seminar, *Polytechnic Institute of New York University*, 1 April 2011.

52. “Computational Structure Prediction and Design of Biomineralization Proteins,” Chemistry Seminar, *University of Maryland Baltimore County*, 29 March 2011.

2010

51. “Computational Structure Prediction and Design of Biomineralization Proteins,” Chemical & Biomolecular Engineering Seminar, *University of Illinois*, 2 November 2010.

50. “Fundamentals and Applications of Protein Structure Prediction,” Program in Computational Biology, *University of Pittsburgh*, 8 October 2010.

49. “Structure Prediction and Design of Biomineralization Proteins,” Faculty of Dentistry Seminar, *McGill University*, 6 May 2010.

48. “Fundamentals and Applications of Protein Structure Prediction,” Anatomy and Cell Biology Department Seminar, *McGill University*, 5 May 2010.

2009

48. “*De novo* computational design of peptide-calcite biomineralization systems,” Symposium on Molecular Biomimetics and Materials Design, *Materials Research Society Fall 2009 Meeting*, Boston, MA, 2 December 2009.

47. “Computational structure prediction and design of biomineralization proteins,” *Gordon Research Conference on Thin Film & Crystal Growth Mechanisms*, New London, NH, 14 July 2009.

46. “Computational structure prediction and design of biomineralization proteins,” *Pacific Northwest National Laboratories*, Richland, WA, 7 May 2009.

45. “Computational structure prediction and design of biomineralization proteins,” *University of Washington*, Physical Chemistry Seminar, 6 May 2009.

2008

44. “Computational structure prediction and design of protein interactions with solid surfaces,” *Beckman Young Investigator Symposium*, Irvine, CA, August 2008.

43. “Motions and communication networks in allosteric proteins,” *National Center for Biotechnology Information* (NCBI), NIH, Bethesda, MD, August 6, 2008.

42. "Computational prediction of structures of protein complexes and multi-domain proteins," *American Crystallographic Association National Meeting*, Knoxville,TN, June 5, 2008.

41. "Fundamentals and applications of protein structure prediction," *University of Texas at Austin,* Chemical Engineering Department Seminar, 18 March 2008.

2007

40. "Fundamentals and applications of protein structure prediction," *Computational Biology Colloquium*, *New York University*, 2 November 2007.

39. "Flexible backbone protein-protein docking with conformer selection and induced fit models," *21st Annual Gibbs Conference on Biothermodynamics*, Carbondale, Illinois, 2 October 2007

38. "Fundamentals and applications of protein structure prediction," *Chemical & Biomolecular Engineering, Johns Hopkins University*, 20 September 2007

37. "Fundamentals and applications of protein structure prediction," *Center for Structural Biology, University of Florida*, 17 September 2007

36. "Flexible backbone protein-protein docking with conformer selection and induced fit models," *JHU Institute for Biophysical Research Annual Retreat*, 15 September 2007

35. "Computational structure prediction of therapeutic antibodies with their antigens," *Biochemical Engineering XV*, Québec City, Canada, 16 July 2007.

34. "Protein-protein docking with applications to therapeutic antibodies," *The Korean Society for Biotechnology and Bioengineering Annual Conference*, Seoul, Korea, 28 April 2007.

33. "Computational Protein Structure Prediction Applied to Docking, Therapeutic Antibodies, and Allostery," *Princeton University*, Chemical Engineering departmental seminar, 14 March 2007.

2006

32. "Protein-Protein Docking applied to Therapeutic Antibodies with their Antigens," *University of California at San Francisco*, Pharmaceutical Sciences and Pharmacogenomics Program Seminar, 15 November 2006.

31. "Local motions and networks in allosteric proteins," *University of Wisconsin Computational Biology Retreat (BACTER),* Madison, WI, 16 September 2006.

30. "Computational Protein Structure Prediction Applied to Docking, Therapeutic Antibodies, and Allostery," *Johns Hopkins University Biophysics departmental seminar*, Baltimore, MD, 17 April 2006.

29. "Computational Protein Structure Prediction Applied to Docking, Therapeutic Antibodies, and Allostery," *Virginia Tech Chemical Engineering departmental seminar*, Blacksburg, VA, 23 January 2006.

28. "Computational Protein Structure Prediction Applied to Docking, Therapeutic Antibodies, and Allostery," *Georgia Institute of Technology, Chemical Engineering departmental seminar*, Atlanta, GA, 11 January 2006.

2005

27. "Prediction of the structure of an anti-cancer therapeutic antibody with its antigen by combining docking with computational and experimental mutagenesis," *JHU Institute for*

Multiscale Modeling of Biological Interactions, 1st Annual Retreat, Towson, MD, 18 November 2005.

26. "Computational Protein Structure Prediction Applied to Docking, Therapeutic Antibodies, and Allostery," *University of Maryland, Baltimore County, Chemical & Biochemical Engineering departmental seminar*, 17 October 2005.

25. "Computational Protein Structure Prediction Applied to Docking, Therapeutic Antibodies, and Allostery," *Michigan State University, "Science at the Edge" seminar series*, Quantitative Biology and Modeling Initiative, 14 October 2005.

24. "Computational Protein Structure Prediction Applied to Docking, Therapeutic Antibodies, and Allostery," *Biogen Idec*, Cambridge, MA, 9 August 2005.

23. "'Truly blind' docking of a novel anti-cancer therapeutic antibody to the epidermal growth factor receptor," *Third conference on Modeling of Protein Interactions in Genomes*, Lawrence, KS, 26 June 2005.

22. "The Prediction of the Structure of Protein-Protein Recognition Sites," *Gordon Research Conference on Structural, Functional & Evolutionary Genomics*, Bates College, Lewiston, ME, 20 June 2005.

21. "Research and Outreach Programs of the Gray Lab," *National Institute of General Medical Sciences*, Bethesda, MD, 16 June 2005 (talk and discussion following Ryan Harrison's win at the Intel Science Talent Search).

20. "Biomolecular Modeling of Therapeutic Antibody Structure & Binding," *Chemical Engineering Department Seminar, University of Maryland at College Park*, May 10, 2005.

19. "What can protein structure prediction do for you?" *JHU Biophysical Evening Series*, Baltimore, MD, February 9, 2005 (with A. Sivasubramanian, M. Daily, & R. Harrison).

2004

18. "Protein-Protein Docking," *George Washington University*, Washington, DC, October 8, 2004.

17. "Protein-Protein Docking," *George Mason University Bioinformatics Colloquium*, Manassas, VA, October 5, 2004.

16. "Rosetta Development: C++ Conversion, Code Modernization, and Benchmarking Issues," *Second Annual Rosetta Developers Conference*, Leavenworth, WA, August 9, 2004.

15. "Progress in Modeling Protein-Protein Docking, Protein Allostery, Protein-Surface Interactions, Therapeutic Antibodies, Protein Electrostatics, and Genomic-scale Interactions" *Second Annual Rosetta Developers Conference*, Leavenworth, WA, August 9, 2004 (with M. Daily, A. Sivasubramanian, D. Masica, G. Lande, T. Upadhyaya & R. Harrison).

14. "Biomolecular Modeling of Protein Interactions," *Data Intensive Science at JHU* (Workshop), Baltimore, June 22, 2004.

13. "Predicting Biomolecular Assembly Through Protein-Protein Docking," *JHU Symposium on Computational Biology, Systems Biology, and Bioinfomatics*, Baltimore, May 24 2004.

12. "Protein-Protein Docking," *NIH Computational Biophysics Section*, Bethesda, MD, May 2004.

11. "Finding the Protein-Protein Interface via Docking Calculations," *Interface 2004*, Baltimore, May 2004.

2002-2003

10. "Protein-Protein Docking Issues in the Gray Laboratory at Johns Hopkins University," *First Annual Rosetta Developers Conference*, Leavenworth, WA, August 2003.

9. "Modeling Protein-Protein Binding: Techniques, Blind Predictions, and Applications to Engineered Antibodies and Biomolecular Switches," *JHU Dept. of Biological Chemistry*, Baltimore, MD, May 2003.

8. "Predicting Protein-Protein Docking," *JHU Institute for Biophysical Research Annual Retreat*, Baltimore, MD, October 2002.

Prior to JHU (2000-2002)

7. "Structure Formation in the Adsorption of Colloidal and Nanoscale Particles," *University of Pennsylvania, Department of Chemical Engineering*, January 24, 2000.

6. "Structure Formation in the Adsorption of Colloidal and Nanoscale Particles," *University of Massachusetts, Department of Chemical Engineering*, February 3, 2000.

5. "Structure Formation in the Adsorption of Colloidal and Nanoscale Particles," *Johns Hopkins University, Department of Chemical Engineering*, February 10, 2000.

4. "Structure Formation in the Adsorption of Colloidal and Nanoscale Particles," *Massachusetts Institute of Technology, Department of Chemical Engineering*, February 18, 2000.

3. "Structure Formation in the Adsorption of Colloidal and Nanoscale Particles," *Northwestern University, Department of Chemical Engineering*, March 9, 2000.

2. "Structure Formation in the Adsorption of Colloidal and Nanoscale Particles," *University of Washington, Department of Chemical Engineering*, March 14, 2000.

1. "Structure Formation in the Adsorption on Colloidal and Nanoscale Particles," *University of California at Berkeley, Department of Chemical Engineering*, March 23, 2000.

IX. Contributed Presentations and Posters

Underline indicates speakers other than Gray. § indicates posters.

2015

108.§ Nance, M., Labonte, J. W. & **Gray JJ**, "Toward the Rational Design of Antibodies with Improved Therapeutic Potential," *Society for Glycobiology Annual Meeting*, San Francisco, 3 December 2015.

107.§ Labonte, J. W. & **Gray JJ**, "RosettaCarbohydrates: Expanding the computational tools available to glycoscientists," *Society for Glycobiology Annual Meeting*, San Francisco, 2 December 2015.

106. Koehler-Leman, J., Alford, R. & **Gray JJ**, "An Integrated Framework Advancing Membrane Protein Modeling and Design," *AIChE Annual Meeting*, Salt Lake City, 10 November 2015.

105. Pacella, M. S., Jiang, W., Athanasiadou, D., Nelea, V., Vali, H., Hazen, R. M., McKee, M.D. & **Gray JJ**, "Modeling chiral recognition between amino acids and vaterite surfaces," *AIChE Annual Meeting*, Salt Lake City, 11 November 2015.

104.§ Weitzner, B., Dunbrack, R. & **Gray JJ**, "The origin of CDR H3 structural diversity," *RosettaCon XIII*, Leavenworth, WA, 31 July 2015. **RosettaCon Best Poster Award.**

103. Labonte, JW & **Gray JJ**, "RosettaCarbohydrates: Expanding the Computational Tools Available to Glycoscientists," *RosettaCon XIII*, Leavenworth, WA, 31 July 2015. **RosettaCon Best Talk Award.**

102.§ Labonte, JW & **Gray JJ**, "Toward structure prediction and design of protein glycosylations," *Biochemical and Molecular Engineering XIX*, Puerto Vallarta, Mexico, 15 July 2015.

101. **Gray JJ**, "Teaching Biomolecular Structure Prediction and Design with PyRosetta," Biochemical and Molecular Engineering Education Workshop, *Biochemical and Molecular Engineering XIX*, Puerto Vallarta, Mexico, 15 July 2015.

100. Weitzner, B., Marze, N., Kuroda, D., Dunbrack, R. & **Gray JJ**, "Producing physically realistic structural models with RosettaAntibody," *Americas Antibody Congress*, San Diego, 27 May 2015.

99.§ Weitzner, B., Dunbrack, R. & **Gray JJ**, "The origin of CDR H3 structural diversity," *Biophysical Society*, Baltimore, MD, 11 February 2015.

98.§ Roy Burman, S. S., Pacella, M., De Yoreo, J. & **Gray JJ**, "Characterization of peptides designed to control crystal nucleation and growth," *Biophysical Society*, Baltimore, MD, 10 February 2015.

97.§ Labonte, J. L. & **Gray JJ**, "Docking and design of oligosaccharides, glycoproteins, and glycolipids," *Biophysical Society*, Baltimore, MD, 10 February 2015.

96.§ Koehler Leman, J., Alford, R. F. & **Gray JJ**, "Rosetta-MPDock: A novel computational tool for protein-protein docking within the membrane bilayer," *Biophysical Society*, Baltimore, MD, 10 February 2015.

2014

95.§ Labonte, J. L. & **Gray JJ**, "Docking and design of oligosaccharides, glycoproteins, and glycolipids: Expanding the computational tools available to glycoscientists," *Joint Meeting of the Society for Glycobiology and the Japanese Society of Carbohydrate Research*, Honolulu, HI, 19 November 2014.

94. **Gray JJ** & Kortemme T, "Computational Molecular Biophysics: Design Your Future," *Grace Hopper Celebration of Women in Computing*, Phoenix, AZ, 8 October 2014.

93.§ Jiang W, Pacella MS, Athanasiadou D, Vali H, **Gray JJ** and McKee MD, "Chiral acidic amino acids induce biomineral chirality: Effects of L- and D- Asp and Glu on calcium carbonate (vaterite) growth," *Gordon Research Conf. on Biomineralization*, New London, NH. August 2014.

92.§ Pacella, M., Roy Burman S. S. & **Gray, J. J.**, "Computational design of peptides to control calcite growth," *Gordon Research Conf. on Biomineralization*, New London, NH. August 2014.

91.§ Roy Burman S. S., Pacella, M., DeYoreo, J. J. & **Gray, J. J.**, "Experimental characterization of peptides to control calcite growth," *Gordon Research Conf. on Biomineralization*, New London, NH. August 2014.

2013

90. Kuroda, D. & **Gray, J. J.**, "Capturing Binding-Induced Conformational Changes in Protein Engineering Calculations," *AIChE Annual Meeting*, San Francisco, CA, 3 November 2013.

89. Weitzner, B. D., Dunbrack, R. L. & **Gray, J. J.**, "Identification of CDR H3-Like Loop Conformations in Non-Immunoglobulin Proteins," *AIChE Annual Meeting*, San Francisco, CA, 6 November 2013.

88. Labonte, J. & **Gray, J. J.**, "Making the most of PyRosetta," *Rosetta Developers Conference*, Leavenworth, WA, 30 July 2013.

87. Lyskov, S. & **Gray, J. J.**, "ROSIE and the testing harness," *Rosetta Developers Conference*, Leavenworth, WA, 30 July 2013.

86. Kuroda, D. & **Gray, J. J.**, "Pushing the backbone in flexible docking," *Rosetta Developers Conference*, Leavenworth, WA, 30 July 2013.

85. Weitzner, B., Dunbrack, R. L. & **Gray, J. J.**, "Antibodies are proteins too!" *Rosetta Developers Conference*, Leavenworth, WA, 28 July 2013.

84.§ Kilambi, K.P. & **Gray, J. J.**, "Cross-docking to identify antibody-antigen interaction partners," *5th CAPRI Evaluation Meeting*, Utrecht, The Netherlands, 19 April 2013.

83. Kilambi, K.P., Pacella, M., Xu, J., Labonte, J. W., Muthu, P., Drew, K., Duroda, D., Scheuler-Furman, O., Bonneau, R. & **Gray, J. J.**, "Blind predictions of structures and binding affinities of protein complexes," *American Chemical Society Annual Meeting*, New Orleans, LA, April 2013.

82. Kilambi, K.P. & **Gray, J. J.**, "Rapid calculation of protein pK_a values using Rosetta," *American Chemical Society Annual Meeting*, New Orleans, LA, April 2013.

2012

81. Masica, D. L., Schrier, S., Specht, E., Sayeg, M. & **Gray, J. J.**, "Design and Prediction of Peptides that Control Biomineralization," *AIChE Annual Meeting*, Pittsburgh, PA, 30 October 2012.

80. Kilambi, K.P. & **Gray, J. J.**, "Rapid calculation of protein pK_a values using Rosetta," *AIChE Annual Meeting*, Pittsburgh, PA, 29 October 2012.

79. Xu, J., & **Gray, J. J.**, "Rosetta-based Computational Pipeline for Antibody Engineering," *Rosetta Developers Conference*, Leavenworth, WA, 1 August 2012.

78.§ Xu, J., Mikos, A. E., Hughes, R., Kuhlman, B., Georgiou, G., Ellington, A. D. & **Gray, J. J.**, "Predict and enhance antibody-antigen binding in the absence of antibody crystal structures: A systematic computational method," *ACS Annual Meeting*, San Diego, CA, 27 March 2012.

77.§ Xu, J., Mikos, A. E., Hughes, R., Kuhlman, B., Georgiou, G., Ellington, A. D. & **Gray, J. J.**, "A systematic computational method to predict and enhance antibody-antigen binding in the absence of antibody crystal structures," *Biophysical Society Annual Meeting*, San Diego, CA, 29 February 2012.

76.§ Kilambi, K.P. & **Gray, J. J.**, "Towards fast and accurate calculation of protein pK_a values exploiting various degrees of conformational flexibility," *Biophysical Society Annual Meeting*, San Diego, CA, 26 February 2012.

2011

75. Kilambi, K.P. & **Gray, J. J.**, "Predicting pKa shifts using the Rosetta score function," *Rosetta Developers Conference*, Leavenworth, WA, 6 August 2011.

74. Lyskov, S., Weitzner, B., & **Gray, J. J.**, "Wrap it up! Communicating between PyRosetta and C++," *Rosetta Developers Conference*, Leavenworth, WA, 6 August 2011.

73.§ Lee, M.-Y., Cao, B., Mao, C. & **Gray, J. J.**, "FD Bacteriophage Coat Protein Structure Prediction and Design for the Assembly of Hydroxyapatite Nanorods and Bone Tissue Regeneration," *Biophysical Society Annual Meeting*, Baltimore, MD, 6 March 2011.

72.§ Kilambi, K.P. & **Gray, J. J.**, "Incorporating the Effects of pH In Protein-Protein Docking," *Biophysical Society Annual Meeting*, Baltimore, MD, 7 March 2011.

71.§ Kilambi, K.P. & **Gray, J. J.**, "Incorporating the Effects of pH In Protein-Protein Docking," *International Conference on Biomolecular Engineering (SBE)*, San Francisco, CA, January 2011.

70.§ Berrondo, M., Chaudhury, S., Muthu, P., Bergman, H. & **Gray, J. J.**, "Improvements to Computational Protein-Protein Docking Methods Allow for the Modeling of a Wider Variety of Biologically Relevant Protein-Protein Interfaces," *International Conference on Biomolecular Engineering (SBE)*, San Francisco, CA, January 2011.

2010

69. **Gray, J. J.**, "How to Teach Protein Structure Prediction and Design," *Rosetta Developers Conference*, Leavenworth, WA, 5 August 2010.

68. Weitzner, B., Lyskov, S., Baugh, E., & **Gray, J. J.**, "A PyMOL-PyRosetta Link: Real-time visualization and feedback for protein structure prediction and design," *Rosetta Developers Conference*, Leavenworth, WA, 4 August 2010.

67. Chaudhury, S. & **Gray, J. J.**, "Identification of Structural Mechanisms of HIV-1 Protease Specificity Using Computational Peptide Docking: Implications for Drug Resistance," *Gordon-Kenan Research Seminar on Biomolecular Interactions and Methods*, Galveston, TX, 17 January 2010.

2009

66. Chaudhury, S., Sircar, A., Kilambi, K. P., & **Gray, J. J.**, "Toward Accurate Homology Model Docking with RosettaDock in CAPRI Rounds 13-19," *4th CAPRI Meeting*, Barcelona, December 2009

65. Chaudhury, S. & **Gray, J. J.**, "Identification of Structural Mechanisms of HIV-1 Protease Specificity Using Computational Peptide Docking: Implications for Drug Resistance," *AIChE Annual Meeting*, Nashville, TN, November 2009.

64. Berrondo, M., **Gray, J. J.**, & Schleif, R. S., "Computational predictions of the mutant behavior of AraC," *AIChE Annual Meeting*, Nashville, TN, November 2009.

63. Berrondo, M. & **Gray, J. J.**, "Loop Modeling in Proteins Using a Conformational Bias Approach," *AIChE Annual Meeting*, Nashville, TN, November 2009.

62. **Gray, J. J.**, Chaudhury, S., & Lyskov, S., "PyRosetta: An Interactive Platform for Teaching Protein Structure Prediction and Design," *AIChE Annual Meeting*, Nashville, TN, November 2009.

61. Masica, D. L., Specht, E. A., Schrier, S., & **Gray, J. J.**, "Rational Design of Peptide-Calcite Biomineralization Systems," *AIChE Annual Meeting*, Nashville, TN, November 2009.

60. Masica, D. L., Ndao, M., Goobes, G., Shaw, W., Drobny, G., & **Gray, J. J.**, "Structure Determination of Biomineral-Associated Proteins Using Combined Structure Prediction and Solid-State NMR," *AIChE Annual Meeting*, Nashville, TN, November 2009.

59. Sircar, A. & **Gray, J. J.**, "Paratope structural optimization during antibody-antigen docking," *American Chemical Society 238th National Meeting*, Washington, DC, 19 August 2009.

58.§ Berrondo, M., **Gray, J. J.**, & Schleif, R. S., "Computational predictions of the mutant behavior of AraC," *Protein Society 21st Annual Symposium*, Boston, MA, 26 July 2009.

57. Berrondo, M. & **Gray, J. J.**, "Computational Predictions of the Enzymatic Activity of Single Deletion Mutants," *SBE's 2nd International Conference on Biomolecular Engineering*, Santa Barbara, CA, 19 January 2009.

2008

56. Masica, D. & **Gray, J. J.**, "High-Resolution Adsorbed and Solution-State Ensembles of a Naturally Evolved Biomineralization Protein: Blind and NMR-Guided Predictions," *AIChE Annual Meeting*, Philadelphia, PA, 20 November 2008.

55. Berrondo, M. Ostermeier, M., & **Gray, J. J.**, "Computational Predictions of the Enzymatic Activity of Single Deletion Mutants," *AIChE Annual Meeting*, Philadelphia, PA, 19 November 2008.

54. Sircar, A., Sivasubramanian, A, Chaudhury, S. & **Gray, J. J.**, "High-Resolution Homology Modeling of Antibody Fv Regions and Application to Antibody-Antigen Docking," *AIChE Annual Meeting*, Philadelphia, PA, 18 November 2008.

53. Sircar, A. & **Gray, J. J.**, "High-resolution homology modeling of antibody F_v regions and application to antibody-antigen docking," *American Chemical Society Annual Meeting*, Philadelphia, PA, 18 August 2008.

52. Berrondo, M. Ostermeier, M., & **Gray, J. J.**, "Prediction of the structure of domain insert proteins from the structures of the individual domains," *American Chemical Society Annual Meeting*, Philadelphia, PA, 17 August 2008.

51.§ Masica, D. & **Gray, J. J.**, "High-resolution solution-state and hydroxyapatite-bound ensembles of human salivary statherin: Blind and NMR-guided predictions," *Gordon Research Conference on Biomineralization*, New London, NH, 11 August 2008.

50. Masica, D. & **Gray, J. J.**, "Solution and adsorbed-state ensembles of biomineralization proteins with RosettaSurface," *Rosetta Developers Conference*, Leavenworth, WA, 23 July 2008.

49. Daily, M. D., & **Gray, J. J.**, "Networks of local and collective motions reveal mechanochemical coupling in a wide variety of allosteric proteins," *Biophysical Society 52nd Annual Meeting*, San Diego, CA, 4 February 2008.

2007

48.§ Chaudhury, S. & **Gray, J. J.**, "Flexible backbone protein-protein docking with conformer selection and induced fit models," *Modeling of Protein Interactions 2007*, Lawrence, KS, 30 September 2007.

47. Sivasubramanian, A., Sircar, A. & **Gray, J. J.**, "Antibody structure prediction and the use of mutagenesis in docking," *Rosetta Developers Meeting Industry Workshop*, Leavenworth, WA, 3 August 2007.

46. Berrondo, M., Ostermeier, M. & **Gray, J. J.**, "Structure prediction of domain insertion proteins from structures of the individual domains," *Rosetta Developers Meeting*, Leavenworth, WA, 3 August 2007.

45. Daily, M. & **Gray, J. J.**, "Rigid-body motion network model for allosteric transitions," *Rosetta Developers Meeting*, Leavenworth, WA, 2 August 2007.

44. Chaudhury, S. & **Gray, J. J.**, "Towards ensemble docking in RosettaDock: Local docking of idealized, energy minimized structures with multiple backbone conformations," *CAPRI Evaluation Meeting*, Toronto, Canada, 21 April 2007.

43.§ Sircar, A., Chaudhury S., Sivasubramanian, A., Berrondo, M. & **Gray, J. J.**, "Integrating experimental information with docking in CAPRI," *CAPRI Evaluation Meeting*, Toronto, Canada, 20-21 April 2007.

42. Daily, M., Upadhyaya, T. & **Gray, J. J.**, "Contact map rearrangements reveal allosteric pathways through protein structure," *Biophysical Society 51st Annual Meeting*, Baltimore, MD, 4 March 2007.

41.§ Sircar, A. & **Gray, J. J.**, "Antibody-Antigen Docking with Simultaneous CDR-H3 Modeling," *Biophysical Society 51st Annual Meeting*, Baltimore, MD, 5 March 2007.

40.§ Masica, D., Makrodimitris, K., Glifort, E. & **Gray, J. J.**, "Design of a Protein-Solid Surface Interface," *Biophysical Society 51st Annual Meeting*, Baltimore, MD, 5 March 2007.

39.§ Chaudhury, S. & **Gray, J. J.**, "Coupling local changes in activation loop conformation with global conformation changes in IRK," *Biophysical Society 51st Annual Meeting*, Baltimore, MD, 6 March 2007.

38.§ Berrondo, M., Ostermeier, M. & **Gray, J. J.**, "Structure Prediction of Engineered Domain-Insert Protein Switches," *Biophysical Society 51st Annual Meeting*, Baltimore, MD, 5 March 2007.

37.§ Masica, D., Makrodimitris, K., Glifort, E. & **Gray, J. J.**, "Design of a Protein-Solid Surface Interface," *International Conference on Biomolecular Engineering*, Coronado, CA, January 2007. ***Poster award winner**

36.§ Berrondo, M., Ostermeier, M. & **Gray, J. J.**, "Structure Prediction of Engineered Domain-Insert Protein Switches," *International Conference on Biomolecular Engineering*, Coronado, CA, January 2007.

2006

35.§ Sivasubramanian, A. & **Gray, J. J.**, "A new protocol for computational structure prediction of therapeutic antibody-antigen interactions," *IBC Antibody Engineering Conference*, San Diego, CA, 10-14 December 2006.

34. Makrodimitris, K. & **Gray, J. J.**, "Modeling statherin structure binding to hydroxyapatite [001] crystal surface," *AIChE National Meeting*, San Francisco, November 2006.

33. Daily, M. & **Gray, J. J.**, "Local motions in allosteric proteins," *AIChE National Meeting*, San Francisco, November 2006.

32. Daily, M. & **Gray, J. J.**, " Local motions and pathways in a benchmark of allosteric proteins," *JHU Institute for Biophysical Research Annual Retreat*, Baltimore, MD, 16 September 2006.

31. Makrodimitris, K. & **Gray, J. J.**, "Modeling statherin structure binding to hydroxyapatite [001] crystal surface," *ACS National Meeting*, San Francisco, 14 September 2006.

30. Sivasubramanian, A. & **Gray, J. J.**, "Protein-protein docking of 14B7-family antibodies binding to the anthrax protective antigen," *ACS National Meeting*, San Francisco, 12 September 2006.

29.§ **Gray, J. J.**, "Design of Specific Protein Interactions with Solid Surfaces," *Beckman Young Investigator Symposium*, Irvine, CA, 25-26 August 2006.

28.§ Daily, M. & **Gray, J. J.**, "Quantitative determination of allosteric motions and mechanisms from a large dataset of allosteric protein structures," *Biophysical Society National Meeting*, Salt Lake City, 21 February 2006.

2005

27. Sivasubramanian, A. Chao, G., Wittrup, K. D. & **Gray, J. J.**, "Computational prediction of mAb 806-EGFR complex structure by combining protein docking with computational and experimental mutagenesis," *AIChE National Meeting*, Cincinnati, November 2005.

26. Harrison, R. M. & **Gray, J. J.**, "Prediction of pKa shifts in proteins using a discrete rotamer search and the Rosetta energy function," *AIChE National Meeting*, Cincinnati, November 2005.

25.§ Daily, M. & Gray, J. J., "Quantitative determination of allosteric motions and mechanisms from a large dataset of allosteric protein structures," ACS National Meeting, Washington, DC, August 2005.

24.§ **Gray, J. J.**, "Design of Specific Protein Interactions with Solid Surfaces," *Beckman Young Investigator Symposium*, Irvine, CA, 26-27 August 2005.

23. Sivasubramanian, A. & **Gray, J. J.**, "Computational prediction of mAb 806-EGFR complex structure using RosettaDock," *ACS National Meeting*, San Diego, March 2005.

2002-2004

22. Daily, M. D., Sivasubramanian, A., Masica, D., Somarouthu, S., Guo, L. & **Gray, J. J.**, "Performance of RosettaDock in CAPRI Rounds 3-5," *Second CAPRI Evaluation Meeeting*, Gaeta, Italy, 8 December 2004.

21. **Gray, J. J.**, D. Baker, "Protein-Protein Docking with RosettaDock," *ACS National Meeting*, Anaheim, March 2004.

20. **Gray, J. J.**, M. Daily, L. Guo, D. Baker, S. Moughon, C. Wang, O. Schueler-Furman "Protein-Protein Docking Predictions with RosettaDock," *Biophysical Society Meeting*, Baltimore, February 2004.

19. Castañeda C. & **Gray, J. J.**, "Predictions of the Docking of an Engineered Antibody to Anthrax Toxin," *AIChE National Meeting*, San Francisco, November 2003.

18.§ Castañeda C. & **Gray, J. J.**,"Predictions of the Docking of an Engineered Antibody to Anthrax Toxin," *Bioengineering XIII*, Boulder, CO, July 2003.

17.§ Castañeda C. & **Gray, J. J.**, "Predictions of the Docking of an Engineered Antibody to Anthrax Toxin," *MABEC 2003*, College Park, MD, March 2003.

16. **Gray, J. J.**, & Baker, D., "Protein-Protein Docking," *AIChE Annual Meeting*, Indianapolis, IN, November 2002.

15. **Gray, J. J.**, Moughon, S., Kortemme, T., Furman, O., Misura, K., Wang, C. & Baker, D. "Protein-Protein Docking Predictions for the CAPRI Experiment," *First CAPRI Evaluation Meeting*, La Londe des Maures, France, September 2002.

1997-2001

14.§ **Gray, J. J.**, Furman, O., & Baker, D. "Protein-Protein Docking using Knowledge-Based Potentials and Monte Carlo Sampling," *Modeling of Protein-Protein Interactions in Genomes*, Charleston, SC, June 2001.

13. **Gray, J. J.**, Klein, D. H., Korgel, B. A. & Bonnecaze, R. T. "Dynamic Non-Equilibrium Phase Behavior During the Random Sequential Adsorption of Tethered Hard Disks," *APS Annual Meeting*, Seattle, WA, March 2001.

12. **Gray, J. J.**, Klein, D. H., Korgel, B. A. & Bonnecaze, R. T. "Adsorption of Tethered Nanoparticles," *AIChE Annual Meeting*, Los Angeles, CA, November 2000.

11. **Gray, J. J.** & Bonnecaze, R. T. "Structure Formation in the Adsorption of Colloidal Mixtures," *AIChE Annual Meeting*, Dallas, TX, November 1999.

10. **Gray, J. J.** & Bonnecaze, R. T. "Electrostatic Double Layer Interactions in Confined Geometries," *AIChE Annual Meeting*, Dallas, TX, November 1999.

9.§ Klein, D. H., **Gray, J. J.**, Bonnecaze, R. T. & Korgel, B. A. "Creation of surface nanostructures by adsorption of tethered nanoparticles," *AIChE Annual Meeting*, Dallas, TX, November 1999.

8. **Gray, J. J.** & Bonnecaze, R. T. "Surface Structures Created by the Adsorption of Colloidal Mixtures," *ACS Colloid and Surface Science Symposium*, Cambridge, MA, June 15, 1999.

7. **Gray, J. J.** "Attractions Between Like-Charged Particles...or Colloidal Cold Fusion?" Separations Research Program Graduate Student Seminar, Austin, TX, July 16, 1999.

6. **Gray, J. J.** & Bonnecaze, R. T. "Rheology and Microstructure of Sheared Arrays of Colloidal Particles," *Society of Rheology Annual Meeting*, Monterey, CA, October 7, 1998.

5. **Gray, J. J.** "Activities of the UT ASEE Student Chapter," *ASEE National Conference*, Seattle, WA, June 1998.

4. **Gray, J. J.** "Rheology and Microstructure of Colloidal Suspensions," Celanese Graduate Student Presentation Competition, Austin, TX, April 1998 (**winner**).

3.§ **Gray, J. J.** "Rheology and Microstructure of Colloidal Suspensions," *Materials Science Summer Institute*, Lakewood, NJ, August 1998.

2. **Gray, J. J.** & Bonnecaze, R. T. "Hysteretic Behavior of Sheared Arrays of Colloidal Particles," *APS Division of Fluid Dynamics Meeting*, San Francisco, CA, November 25, 1997.

1. Matsumoto, E., Tumer, I. Y., Arthur, L. F. & **Gray, J. J.** "How to Establish an ASEE Student Chapter," *ASEE National Conference*, Milwaukee, WI, June 1997.

X. Professional Activities

Editorial service:

Editorial Board, Proteins: Structure, Function, and Bioinformatics, 2004-present
Guest editorial manager, Proteins: Structure, Function, Genetics, 2003-2004

Meetings organized:

Conference co-chair, Fourth Annual Rosetta Developers Conference, Leavenworth, WA, July 2006 (with Prof. Brian Kuhlman).
Conference co-chair, Third Annual Rosetta Developers Conference, Leavenworth, WA, July 2005 (with Prof. Carol Rohl).
Conference co-chair, Second Annual Rosetta Developers Conference, Leavenworth, WA, August 2004 (with Prof. Carol Rohl).

Sessions chaired:

Session co-chair, "Protein Aggregation, Engineering, and Design," ECI Biochemical and Molecular Engineering, Cabo San Lucas, 12-16 July 2015 (with Prof. Michelle O'Malley and Dr. Dana Andersen).
Session chair, "Gender and Science," Eleventh Annual Rosetta Conference, Leavenworth, WA, 1 August 2014.
Session co-chair, "Biomolecular and Biophysical Processes: Assembly, Stability, and Engineering in Model Protein Systems," American Chemical Society Annual Meeting, New Orleans, April 2013 (with Dr. Parag Kolhe)
Session co-chair, "Protein Engineering," American Institute of Chemical Engineers Annual Meeting, Nashville, November 2009 (with Prof. Patrick Cirino)
Session co-chair, "Computational and experimental tools for the design and engineering of biomolecules," First International Conference on Biomolecular Engineering, Coronado Island, CA, January 2007 (with Prof. Eric Boder).
Session co-chair, "Advances in Protein Structure, Function, and Stability," American Institute of Chemical Engineers Annual Meeting, San Francisco, November 2006 (with Prof. Christopher J. Roberts)
Session chair, "Protein-Protein Interactions," American Chemical Society Annual Meeting, San Francisco, CA, September 2006 (with Dr. Alexey Lugovskoy).
Session chair, "Advances in Protein Structure, Function, and Stability," American Institute of Chemical Engineers Annual Meeting, Cincinnati, OH, November 2005 (with Prof. Christopher J. Roberts)
Session chair, "Design of Core Objects in Rosetta," Third Annual Rosetta Developers Conference, Leavenworth, WA, July 2005.
Session co-chair, "Protein Folding and Characterization," American Chemical Society Annual Meeting, San Diego, CA, March 2005 (with Dr. Bruce Kerwin).
Session chair, "Advances in Protein Structure, Function, and Stability," American Institute of Chemical Engineers Annual Meeting, Austin, TX, November 2004 (with Prof. Christopher J. Roberts)
Poster session co-chair, "Fluid Mechanics Poster Session," American Institute of Chemical Engineers Annual Meeting, Reno, NV, November 2002 (with Prof. Surita Bhatia)

Proposal reviewing:

NSF panel member, Systems and Synthetic Biology (SSB), Molecular and Cellular Biology (MCB), February 2014

NSF CAREER panel member, Biotechnology, Biochemical and Biomass Engineering (BBBE), October 2012
NSF panel member, Biotechnology, Biochemical and Biomass Engineering (BBBE) unsolicited proposal panel, June 2009
NIH *ad hoc* study section member:
Macromolecular Structure and Function B (MSFB), Oct. 2008
Computational Molecular Biophysics (BCMB-Q), June 2006
Quantitative Biological Structure (BST-D), 2004
Reviewed miscellaneous proposals for NIH, NSF, ACS-PRF, Jeffress Trust, Netherlands Organization for Scientific Research, Vanderbilt IDEAS

Manuscript reviewing:

Science, Proc. Natl. Acad. Sci. U.S.A., Proteins, *J. Mol. Biol.*, *J. Am. Chem. Soc., PLoS Comput. Biol., Biophys. J.*, *Protein Science*, *Structure*, *Nucleic Acids Res.*, *Nature Methods, Nature Nanotechnol.*, *Macromolecules*, *Langmuir*, *J. Comp. Chem.*, *J. Colloid Interface Sci., Immunome Res., Bioinformatics, PLoS One, Protein Eng. Des. & Selection, Chem. Eng. Sci.*, *J. Struct. Biol.*, *others*

Professional society membership:

American Institute of Chemical Engineers, Senior Member
- Faculty advisor to the JHU student chapter (see §XIII), 2003-2008

American Society for Engineering Education
- Founding Member of UT Student Chapter, 1996
- UT Student Chapter President, 1997-1998

American Chemical Society
Biophysical Society
Society for Biological Engineering

Community and business leadership:

Board of Directors, Ingenuity Project, Baltimore, 2005-2015.
Non-profit, accelerated math and science program with the Baltimore City Public School System.
- Co-founded RAMP, an after-school robotics program for Mt. Royal Middle School Students organized by JHU ChemBE undergraduates (2010-2011)

Scientific Advisory Board, Rosetta Design Group LLC, Washington DC, 2007-present
Macromolecular modeling services with the Rosetta software suite to support the pharmaceutical and biotechnology industries.

Diversity Chair, Rosetta Commons, 2014-present.
- Responsible for diversity and inclusion in 40-lab Rosetta collaboration.
- Organized delegation to attend Grace Hopper Celebration of Women in Computing
- Code of Conduct review panel, responsible for evaluating and responding to conduct reports.
- Created an intern program, secured NSF funding, and recruited diverse class.

Consulting:

Legal consultant for pharmaceutical patent case, 2015.

XI. Software and Electronic Resources Provided

Our lab co-develops the **Rosetta protein structure prediction and design suite** in collaboration with 41 other Rosetta developing labs. Our lab is the prime developer of:
RosettaDock (protein-protein docking),
RosettaSurface and **RosettaSurface.Design** (protein-solid surface docking and design),

RosettaAntibody (high-resolution antibody homology modeling),
EnsembleDock (conformer-selection docking),
SnugDock (antibody docking),
RosettaCarbohydrate and others.

Rosetta has been distributed for free to over 19,000 licensees. Revenues of over $800,000/yr raised from commercial licenses from over 50 companies, 2002-present, *http://www.rosettacommons.org.*

PyRosetta libraries for interactive protein structure prediction and design, *http://pyrosetta.org*. Since 2010, over 2,200 licensees including 7 companies (see publications #33 & #47).

ROSIE, the Rosetta Online Server that Includes Everyone, a unified server providing access to diverse Rosetta protocols (see publication #54). Over 2,400 jobs completed since December 2012. *http://rosie.graylab.jhu.edu*

RosettaDock Protein-Protein Docking Server, over 10,000 jobs completed 2007-2012 (see publication #24), now superseded by ROSIE.

RosettaAntibody Structure Prediction Server, over 2,400 jobs completed 2008-2012 (see publication #29), now superseded by ROSIE.

Allosteric protein structure database, 2006, *http://graylab.jhu.edu/allostery*

Protein-protein docking decoy sets for testing biomolecular energy functions, 2002, *http://graylab.jhu.edu/docking/decoys*

XII. University, School of Engineering, and Programmatic Service

University Committees and Service:

Diversity Leadership Council, 2013-2016
- Chair, Faculty Recruitment and Development Subcommittee, 2013-present
- Member, Family Support Subcommittee, 2013-present

Provost's Task Force on Mentoring, 2015-2017
SABES Faculty Outreach Oversight Committee, 2012-present
- Interim Director, Summer 2014

Faculty Committee on Admissions, 2008-2011
Academic Computing Advisory Committee, 2005-2012
JHU Undergraduate Open House Panel Member, 2006

Whiting School of Engineering Committees:

Whiting School of Engineering Information Technology Committee, 2013-present
Whiting School of Engineering Centennial Committee, 2012-2013
Whiting School of Engineering Education Innovation Vision Committee, 2011-2012
WSE EDIT/FOLIO Data System Upgrade Committee, 2009-2010
Whiting School of Engineering Teaching Award Selection Committee, 2007
Vredenburg Scholarship Selection Committee, 2006, 2007

Programmatic Service:

Program in Molecular Biophysics Steering Committee, 2013-Present
Program in Molecular & Computational Biophysics Thesis Review Committee, 2005-2008
Institute for Computational Medicine Faculty Search Committee, 2005-2006

Thesis Committees:

Doctoral Thesis Committee Member (10 students 2002-2012)
Graduate Board Oral Exam Committee Member (20 students, 2002-2011)

XIII. Departmental Service

Leadership:

Director of Graduate Admissions, 2011-2012; 2013-2015
Director of Alumni and Development, 2011-present
Director, Hopkins ChemBE Career Network, 2008-2011
Senior Editor, *ChemBE Bond* (alumni newsletter), 2009-2011
Coordinator, Graduate Student Thesis Reviews (pilot), 2007-2008
Chair, Seminar Series, 2005-2007
Advisor to the AIChE/SBE Student Chapter, 2003-2008

- National Winner of the Senior Sign-Up Contest, 2008
- AIChE chapter relaunched as a joint AIChE/SBE chapter in 2007

Coordinator, Elenora Streb Muly Undergraduate Research Scholarship Program, 2004-2008

Events organized:

Alumni Receptions at AIChE National Meetings, 2012-present
1st and 2nd Annual ChemBE Undergraduate Poster Session, May 2005-2006
AIChE Maryland Chapter meeting at JHU featuring talks by ChemBE graduate students, 2004 and 2006
ChemBE Research Symposium, 2008, with Undergraduate Poster Session and AIChE Maryland Chapter meeting featuring talks by ChemBE graduate students (with Prof. Dilip Asthagiri)
Departmental service project at Coleman Elementary School, MLK Day 2004

Departmental committees:

Faculty Search Committee Diversity Advocate, 2015-2016
Undergraduate Curriculum Committee, 2014
ABET Committee, 2009-2010
Graduate Admissions Committee, 2005
Kinetics Qualifier Exam committee, 2003-2004, 2006-2009
Thermodynamics Qualifier Exam committee, 2005
NSF-REU selection committee, 2003
Departmental computing curriculum committee member, 2006, 2008

Graduate student committees:

Doctoral Thesis Committee Member (7 students, 2002-2012)
Graduate Board Oral Exam Committee Member (6 students, 2002-2012)
Masters Thesis Committee Member (6 students, 2002-2012)
Thesis Review Committee Member (1 student, 2008)

XIV. Outreach

<u>Rosetta Diversity Chair</u>
Led a delegation of Rosetta developers and PIs to attend, present, and recruit at the 2014 & 2015 Grace Hopper Celebration of Women in Computing (Phoenix, AZ & Houston, TX). Created an NSF-funded REU program across Rosetta labs (Summer 2015-2016), see *rosettacommons.org/intern*.

Member of a panel that responds to reports under the Rosetta Commons Code of Conduct. This panel works to ensure a welcoming and inclusive scientific environment.

Organized plenary sessions at the Rosetta Conference and the Developers Conferences around themes of diversity and inclusion.

Ingenuity Project
The Ingenuity Project is a non-profit organization operating within the Baltimore City Public School System that aims to prepare highly capable and motivated Baltimore students to achieve at nationally competitive levels in mathematics and science. Ingenuity currently serves over 500 students in grades 5-12 at four different Baltimore City public schools; the demographics include 47% African-Americans and 52% girls/young women. I have served on the Board of Directors since 2005. I mentored Ryan Harrison, 5th place winner of the Intel Science Talent Search in 2005. Harrison was the first winner from Baltimore city in over 40 years and was the only African-American winner in the decade; he has subsequently earned his Ph.D. in Chemistry.

STEM Achievement in Baltimore Elementary Schools, SABES, 2012-present
Faculty participant and member of the faculty outreach oversight board (FOOB) for SABES. SABES is a $7.4M 5-year NSF-funded project that aims to boost STEM education for 3rd-5th grade students in specific Baltimore City neighborhoods. The purpose of the FOOB is to make outreach activities more visible and to provide evidence regarding the broader impact of faculty work in the community.

Members from my lab and a partner lab (Chao Wang) visit a target elementary school weekly during the school year. In 2013-2014, we served the 3rd grade class at John Ruhrah Elementary/Middle School, and in 2014-2015, we serve the 3rd grade class at Dallas F. Nicholas Elementary/Middle School.

Lectures and Activities
Visit to Ingenuity Project 10th Graders at Baltimore Polytechnic Institute, 18 Sept 2009

Engineering Innovation (summer high school program), Hands-on Special Topics Event: “Protein Design with FoldIt!”, Summer 2009, 2010, 2011, 2012, 2013

XV. Teaching (Evaluations range 1-5, 1=low, 5=high)

540.101 Chemical Engineering in Today’s World (1 cr)

	Enrollment	Overall Quality
Fall 2002	23	3.84

540.202 Introduction to Chemical and Biomolecular Processes

	Enrollment	Teaching Effectiveness	Overall Quality	Intellectual Challenge
Fall 2015	68	3.64	4.02	4.26
Spring 2015	33	4.06	4.25	4.00
Spring 2014	35	3.24	3.38	4.21
Fall 2012	45	3.92	4.05	4.61
Fall 2011	37	3.75	4.14	4.43

540.416/616 Current Topics in Protein Structure Prediction (new course)

	Enrollment	Teaching Effectiveness	Overall Quality	Intellectual Challenge
Fall 2012	7	(no statistics for enrollment under 8)		

Fall 2010	8	5.00	4.88	4.62

540.414/614 Computational Protein Structure Prediction and Design (new course)

	Enrollment	Teaching Effectiveness	Overall Quality	Intellectual Challenge
2016 Spring	11	4.80	4.60	4.80
2014 Fall	12	4.55	4.55	4.73
2012 Spring	16	4.40	4.40	4.53
2010 Spring	15	4.70	4.50	4.70
2009 Spring	11	4.45	4.45	4.64

540.460/660 Computational and Experimental Design of Biomolecules (new course)
(co-taught w/Marc Ostermeier)

.

	Enrollment	Teaching Effectiveness	Overall Quality	Intellectual Challenge
2008 Spring	13	4.45	4.55	4.27
2007 Spring	28	3.89	3.95	4.05

540.406/606 Molecular Simulations & Multiscale Modeling (new course)
(co-taught w/German Drazer)

	Enrollment	Teaching Effectiveness	Overall Quality	Intellectual Challenge
2008 Spring	7	4.20	4.20	4.80
2007 Spring	16	4.18	3.90	4.18

540.409 **Modeling, Dynamics & Control of Chemical & Biological Systems** (updated course)

	Enrollment	Teaching Effectiveness	Overall Quality	Intellectual Challenge
2010 Fall	82	4.28	4.25	4.28
2009 Fall	87	4.18	4.12	4.24
2008 Fall	57	3.61	3.63	4.20
2007 Fall	68	3.91	4.04	4.17
2006 Fall	48	4.03	3.82	4.24
2005 Fall	37	4.48	4.40	4.47
2004 Fall	27	4.43	4.24	4.14
2003 Fall	23	-	3.72	-
2003 Spring	16	-	4.07	-

(Before 2004, the questionnaire did not include teaching effectiveness or intellectual challenge.)

Lectures at JHU:

Seminar for “Intro. to Biomedical Research and Careers,” SPH course (Spring 2011)
Lectures for “Methods in Biophysics,” KSAS course (Spring 2010, 2011, 2012)
Lectures for “Multiscale Modeling of Biological Interactions,” IMMBI course (Spring 2006)
Guest lectures for “Protein Bioinformatics” course at SPH (Spring 2004, 2005, 2006)
Guest lecture on protein docking for “Bioinformatics” course in Biophysics (Spring 2004)
Guest lecture on biomolecular modeling for “ChemBE in Today’s World” (Fall 2003)

Other at JHU:

Academic Advisor to part of the ChemBE Class of 2018, 2014-present, 36 students
Academic Advisor to part of the ChemBE Class of 2014, 2010-2014, 25-30 students
Academic Advisor to part of the ChemBE Class of 2010, 2006-2010, 35-40 students
Academic Advisor to the ChemBE Class of 2006, 2002-2006, 20-25 students
Co-leader of the Computational Biophysics Journal Club (with Tom Woolf), 2005-2010

XVI. Recent Collaborators

Within Hopkins:

Prof. James Berger, Biophysics and Biophysical Chemistry (SoM)
Prof. Aravinda Chakravarti, Center for Complex Disease Genomics (SoM)
Prof. Phil Cole, Pharmacology (SoM)
Prof. Karen Fleming, Biophysics
Prof. Marc Ostermeier, Chemical & Biomolecular Engineering
Prof. James Stivers, Pharmacology & Molecular Sciences (SoM)

Outside Hopkins:

Prof. Richard Bonneau, Biology, New York University
Prof. Rhiju Das, Biophysics, Stanford
Prof. James De Yoreo, Pacific Northwest National Laboratory and University of Washington
Prof. Gary Drobny, Chemistry, University of Washington
Dr. Roland Dunbrack, Fox Chase Cancer Research Center, Philadelphia
Prof. Andrew Ellington, University of Texas at Austin
Prof. Ora Scheuler-Furman, Hebrew University, Israel
Prof. George Georgiou, University of Texas at Austin
Prof. Gil Goobes, Chemistry, Bar-Ilan University, Israel
Prof. Robert Hazen, Carnegie Institution for Science, Washington, DC
Prof. Tanja Kortemme, Bioengineering, UCSF
Prof. Brian Kuhlman, Biochemistry, University of North Carolina
Prof. Marc D. McKee, Dentistry, McGill University, Canada
Prof. Jens Meiler, Chemistry, Vanderbilt University
Dr. Wendy Shaw, Chemistry, Pacific Northwest National Laboratory, Washington
Prof. Vladimir Yarov-Yarovoy, University of California at Davis