

Most Cited Research Publications of Warshel Group (Oct., 2007)

I. Research Papers

1200 or Above

- Theoretical Studies of Enzymatic Reactions: Dielectric Electrostatic and Steric Stabilization of the Carbonium Ion in the Reaction of Lysozyme, A. Warshel and M. Levitt, *J. Mol. Biol.* 103, 227-249 (1976). [1205]

700 or Above

- Calculations of Electrostatic Interactions in Biological Systems and in Solutions, A. Warshel and S. T. Russell, *Quart. Rev. Biophys.* 17, 283-422 (1984). [756]

500 or Above

- Calculation of Ground and Excited State Potential Surfaces of Conjugated Molecules. I. Formulation and Parameterization, A. Warshel and M. Karplus, *J. Am. Chem. Soc.* 94, 5612 (1972).[527]

Between 400-499

- A Consistent Force Field for Calculation on Conformations, Vibrational Spectra and Enthalpies of Cycloalkanes and n-Alkane Molecules, S. Lifson and A. Warshel, *J. Chem. Phys.* 49, 5116 (1968). [489]
- Computer Simulation of Chemical Reactions in Enzymes and Solutions, A. Warshel, John Wiley & Sons, (1991). [373]

Between 300-399

- Computer Simulations of Protein Folding, M. Levitt and A. Warshel, *Nature* 253, 694 (1975). [373]
- Q-Chem 2.0: A High-Performance Ab Initio Electronic Structure Program Package: J. Kong, C. A. White, A. I. Krylov, D. Sherrill, R. D. Adamson, T. R. Furlani, M. S. Lee, A. M. Lee, S. R. Gwaltney, T.R. Adams, C. Ochsenfeld, A. T. B. Gilbert, G.S. Kedziora, V. A. Rassolov, D. R. Maurice, N. Nair, Y. Shao, N. A. Besley, P. E. Maslen, J. P. Dombroski, H. Daschel, W. Zhang, P. P. Korambath, J. Baker, E.F. C. Byrd, T. Van Voorhis, M. Oumi, S. Hirata, C-P. Hsu, N. Ishikawa, J. Florian, A. Warshel, B. G. Johnson, P. M. W. Gill, M. Head-Gordon and J. A. Pople, *Journal of Computational Chemistry* 21, 1532-1548 (2000). [371]
- Simulation of Enzyme Reactions Using Valence Bond Force Fields and Other Hybrid Quantum/Classical Approaches, J. Åqvist and A. Warshel, *Chem. Rev.* 93, 2523 (1993). [343]
- Electrostatic Energy and Macromolecular Function. A. Warshel and J. Åqvist, *Ann. Rev. Biophys. Biophys. Chem.* 20, 267 (1991). [340]
- Consistent Force Field Calculations. II. Crystal Structure, Sublimation Energies, Molecular and Lattice Vibrations, Molecular Conformations and Enthalpies of Alkanes, A. Warshel and S. Lifson, *J. Chem. Phys.* 53, 582 (1970). [326]

- How do Serine Proteases Really Work? A. Warshel, G. Naray-Szabo, F. Sussman and J-K. Hwang, *Biochemistry* 28, 3629 (1989). [304]
- An Empirical Valence Bond Approach for Comparing Reactions in Solutions and in Enzymes, A. Warshel and R. M. Weiss, *J. Am. Chem. Soc.* 102, 6218 (1980).[300]

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- Calculations of Chemical Processes in Solutions, A. Warshel, *J. Phys. Chem.* 83, 640 (1979). [284]
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- Energetics of Enzyme Catalysis, A. Warshel, *Proc. Natl. Acad. Sci. USA* 75, 5250 (1978). [253]
- What are the Dielectric “Constants” of Proteins and How to Validate Electrostatic Models?, C.N. Schutz and A. Warshel, *PROTEINS Structure, Function and Genetics*, 44, 400-417 (2001).[248]
- Microscopic and Semimicroscopic Calculations of Electrostatic Energies in Proteins by the POLARIS and ENZYMIK Programs, F. S. Lee, Z. T. Chu, and A. Warshel, *J. Comp. Chem.* 14,161 (1993).[230]
- Macroscopic Models for Studies of Electrostatic Interactions in Proteins: Limitations and Applicability, A. Warshel, S. T. Russell and A. K. Churg, *Proc. Natl. Acad. Sci. USA* 81, 4785 (1984).[220]
- Microscopic Examination of Free Energy Relationships for Electron Transfer in Polar Solvents, J-K. Hwang and A. Warshel, *J. Am. Chem. Soc.* 109, 715 (1987).[215]
- A Surface Constrained All-Atom Solvent Model for Effective Simulations of Polar Solutions, G. King and A. Warshel, *J. Chem. Phys.* 91, 3647 (1989). [213]
- Extreme Conformational Flexibility of the Furanose Ring in DNA and RNA, M. Levitt and A. Warshel, *J. Am. Chem. Soc.* 100, 2607 (1978). [213]
- Calculation of $\pi\pi^*$ Excited State Conformations and Vibronic Structure of Retinal and Related Molecules, A. Warshel and M. Karplus, *J. Am. Chem. Soc.* 96, 5677 (1974). [212]
- Electrostatic Basis of Structure-Function Correlation in Proteins, A. Warshel, *Acc. Chem. Res.* 14, 284 (1981). [211]
- Calculations of Resonance Raman Spectra of Conjugated Molecules, A. Warshel and P. Dauber, *J. Chem. Phys.* 66, 5477 (1977). [208]
- Simulation of Free Energy Relationships and Dynamics of S_N2 Reactions in Aqueous Solutions, J-K Hwang, G. King, S. Creighton and A. Warshel. *J. Am. Chem. Soc.* 110, 5297 (1988). [206]
- On Low-Barrier Hydrogen Bonds and Enzyme Catalysis, A. Warshel, A. Papazyan and P. A. Kollman, *Science* 269, 102 (1995).[204]
- Spectroscopic Properties of Photosynthetic Reaction Centers. 2. Application of the Theory of Rhodopseudomonas Viridis, W. W. Parson and A. Warshel, *J. Am. Chem. Soc.* 109, 6152 (1987). [200]

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- Electrostatic Origin of the Catalytic Power of Enzymes and the Role of Preorganized Active Sites, A. Warshel, Mini Review, *J. Biol. Chem.*, 273, 27035-27038 (1998).[198]

- Calculations of Electrostatic Energies in Proteins; The Energetics of Ionized Groups in Bovine Pancreatic Trypsin-Inhibitor, S.T. Russell and A. Warshel, *J. Mol. Biol.* 185, 389-404 (1985). [197]
- Electrostatic Control of Charge Separation in Bacterial Photosynthesis, W.W. Parson, Z. T. Chu, and A. Warshel, *Biochim. Biophys. Acta.* 1017, 251 (1990). [196]
- Investigation of the Free Energy Functions for Electron Transfer Reactions, G. King and A. Warshel, *J. Chem. Phys.* 93, 8682 (1990). [194]
- Interpretation of Resonance Raman Spectra of Biological Molecules, A. Warshel, *Ann. Rev. Biophys. Bioeng.* 6, 273 (1977).[190]
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- Electrostatic Effects in Macromolecules: Fundamental Concepts and Practical Modeling, A. Warshel and A. Papazyan, *Curr. Opin. Struct. Biol.* 8, 211-217 (1998).[156]
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