Referred Papers

1. X. Yu, J. Yang, Q. Wang, S. Cheng, Ruth Nussinov, and **Jie Zheng***, "Intrinsic twisting and bending properties of soluble beta-sheet-rich self-assemblies: implication for amyloid structures", (submitted to *J. Mol. Bio*.)
2. X. Yu, Q. Wang, J. Yang, I. Buch, C. Tsai, B. Ma, S. Cheng, R. Nussinov, and **Jie Zheng***, "Mutational analysis and allosteric effects in the HIV-1 capsid protein carboxyl-terminal dimerization domain", *Biomacromolecules* 10: 390 (2009)
3. L. Li and **Jie Zheng***, "Computational modeling of amyloid oligomeric structures", *International Journal of Liquid State Sciences*, (in press)
4. **Jie Zheng***, H. Jang, and R. Nussinov, "β_2-microglobulin amyloid fragment organization and morphology and its comparison to Aβ suggests that amyloid aggregation pathways are sequence specific", *Biochemistry* 47: 2497 (2008)
5. **Jie Zheng***, H. Jang, B. Ma, and R. Nussinov, "Annular structures as intermediates in fibril formation of alzheimer Abeta17-42", *J. Phys. Chem. B*, 112: 6856 (2008)
6. **Jie Zheng***, B. Ma, Y. Chang, and R. Nussinov, "Molecular dynamics simulations of Alzheimer's peptide Aβ40 elongation and lateral association", *Frontiers in Bioscience* 13: 3919 (2008)
7. H. Jang, **Jie Zheng**, R. Lal, and R. Nussinov, "New structures help the modeling of toxic amyloid-beta ion channels", *Trends in Biochemical Sciences* 33: 91 (2008)
8. Y. He, Y. Chang, J. Hower, **Jie Zheng**, S. Chen, and S. Jiang, "Origin of repulsive force and structure/dynamics of interfacial water in OEG–protein interactions: a molecular simulation study", *Phys. Chem. Chem. Phys,* 10: 5539 (2008)
9. **Jie Zheng**, B. Ma, H. Jang, C. Tsai, and R. Nussinov, "Modeling the alzheimer Aβ17-42 fibril architecture: tight intermolecular sheet-sheet association and intramolecular hydrated cavities", *Biophysical J.* 93: 3046 (2007)
10. **Jie Zheng**, D. Zanuy, N. Haspel, C. Tsai, C. Aleman, and R. Nussinov, "Nanostructure design using protein building blocks enhanced by conformationally constrained synthetic residues", *Biochemistry* 46: 1205 (2007).
11. H. Jang, **Jie Zheng**, and R. Nussinov, "Models of β-amyloid ion-channels in the membrane suggest that channel formation in the bilayer is a dynamic process", *Biophysical J.* 93: 1938 (2007)
12. C. Tsai**, Jie Zheng**, D. Zanuy, N. Haspel, H. Wolfson, C. Aleman, and R. Nussinov, "Principles of nanostructure design with protein building blocks", *Proteins* 68: 1 (2007)
13. B. Ma, Y. Pan, **Jie Zheng**, A. Levine, and R. Nussinov, "Sequence analysis of p53 response-elements suggests multiple binding modes of the p53 tetramer to DNA targets", *Nucleic Acids Research* 35: 2986 (2007)
14. N. Haspel, D. Zanuy, **Jie Zheng**, C. Aleman, H. Wolfson, and R. Nussinov, "Changing the charge distribution of β-helical based nanostructures can provide the conditions for charge transfer", *Biophysical J.,* 93: 245 (2007)
15. D. Zanuy, F. Rodriguez-Ropero, N. Haspel, **Jie Zheng**, R. Nussinov, and C. Aleman, "Stability of tubular structures based on β-helical proteins: self-assembled versus polymerized nanoconstructs and wild-type versus mutated sequences", *Biomacromolecules* 8: 3135 (2007)

16. **Jie Zheng**, B. Ma, and R. Nussinov "Consensus features in amyloid fibrils: sheet-sheet recognition via a (polar or nonpolar) zipper structure", *Phys. Biol.* 3: P1 (2006)
17. **Jie Zheng**, Y. He, S. Chen, L. Li, M. Bernards, and S. Jiang, "Molecular simulation studies of the structure of phyosphorylcholine self-assembled monolayers", *J. Chem. Phys.* 125: 174714 (2006).
18. **Jie Zheng**, B. Ma, C. Tsai, and R. Nussinov, "Structural stability and dynamics of an amyloid-forming peptide GNNQQNY from yeast prion sup-35", *Biophysical J.,* 91: 824 (2006).
19. C. Tsai, **Jie Zheng**, and R. Nussinov, "Designing a nanotube using naturally occurring protein building blocks", *PLoS Computational Biology* 4: e42 (2006)
20. C. Tsai, **Jie Zheng**, C. Aleman, and R. Nussinov, "Structure by design: From single proteins and their building blocks to nanostrctures", *Trends in Biotechnology* 10: 449 (2006)
21. C. Aleman, D. Zanuy, A. I. Jiménez, C. Cativiela, N. Haspel, **Jie Zheng**, J. Gasanovas, H. Wolfson, and R. Nussinov, "Concepts and schemes for the re-engineering of physical protein modules: generating nanodevices via targeted replacements with constrained amino acids", *Phys. Biol.* 3: S54 (2006)
22. **Jie Zheng**, L.Li, H. Tsao, Y. Sheng, S. Chen, and S. Jiang, "Strong repulsive forces between protein and oligo (ethylene glycol) self-assembled monolayers: a molecular simulation study", *Biophysical J.*， 89: 158 (2005)
23. **Jie Zheng**, E. Lennon, H. Tsao, Y. Sheng, and S. Jiang, "Transport of a liquid water and methanol mixture through carbon nanotubes under a chemical potential gradient", *J. Chem. Phys.,* 122: 214702 (2005)
24. S. Chen, **Jie Zheng**, L. Li, and S. Jiang, "Strong resistance of phosphorylcholine self-assembled monolayers to protein adsorption: insights into nonfouling properties of zwitterionic materials", *J. Am. Chem. Soc.* 127: 14473 (2005)
25. L. Li, S. Chen**, Jie Zheng**, B. D. Ratner, and S. Jiang. "Protein adsorption on oligo(ethylene glycol)-terminated alkanethiolate self-assembled monolayers: the molecular basis for nonfouling behavior", *J. Phys. Chem. B* 109: 2934 (2005)
26. **Jie Zheng**, L. Li, S. Chen, and S. Jiang "Molecular simulation study of water interactions with oligo (ethylene glycol)-terminated alkanethiol self-assembled monolayers", *Langmuir,* 20: 8931 (2004)
27. J. Zhou, **Jie Zheng**, and S. Jiang, "Molecular simulation studies of orientation and conformation of cytochrome c adsorbed on self-assembled monolayers", *J. Phys. Chem. B* 108: 17418 (2004)
28. **Jie Zheng**, R. Balasundaram, S.H. Gehrke, G.S. Heffelfinger, W.A. Goddard III, and S. Jiang, "Cell multipole method for molecular simulations in bulk and confined systems," *J. Chem. Phys.* 118: 5347 (2003)
29. Q. Zhang, **Jie Zheng**, A. Shevade, L. Zhang, S.H. Gehrke, G.S. Heffelfinger, and S. Jiang, "Transport diffusion of liquid water and methanol through membranes", *J. Chem. Phys.* 117: 808 (2002)