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[J. Chem. Phys. 142, 055101 \(2015\)](#)

Probing the folded state and mechanical unfolding pathways of T4 lysozyme using all-atom and coarse-grained molecular simulation

Wenjun Zheng, Paul Glenn
[J. Chem. Phys. 142, 035101 \(2015\)](#)

Systematic characterization of protein folding pathways using diffusion maps: Application to Trp-cage miniprotein

Sang Beom Kim, Carmeline J. Dsilva, Ioannis G. Kevrekidis, Pablo G. Debenedetti
[J. Chem. Phys. 142, 085101 \(2015\)](#)

Aspects of structural landscape of human islet amyloid polypeptide

Jianfeng He, Jin Dai, Jing Li, Xubiao Peng, Antti J. Niemi
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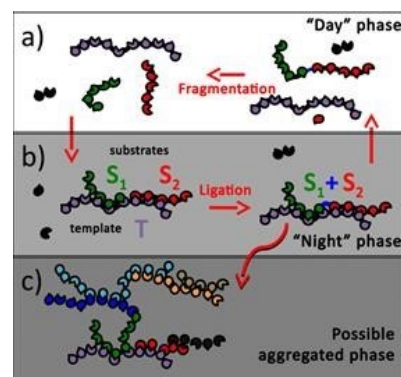
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Spontaneous emergence of

Microscopic dynamics of water around unfolded structures of barstar at room temperature

Somedatta Pal, Kaushik Chakraborty, Prabir Khatua, Sanjoy Bandyopadhyay
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Machine learning of single molecule free energy surfaces and the impact of chemistry and environment upon structure and dynamics

Rachael A. Mansbach, Andrew L. Ferguson
[J. Chem. Phys. 142, 105101 \(2015\)](#)

Water organization between oppositely charged surfaces: Implications for protein sliding along DNA

Amir Marcovitz, Aviv Naftaly, Yaakov Levy
[J. Chem. Phys. 142, 085102 \(2015\)](#)

Dependence of FRET efficiency on distance in single donor-acceptor pairs

I. S. Osad'ko
[J. Chem. Phys. 142, 125102 \(2015\)](#)

Nonlinear vs. linear biasing in Trp-cage folding simulations

Vojtěch Spiwok, Pavel Oborský, Jana Pazúriková, Aleš Křenek, *et al.*
[J. Chem. Phys. 142, 115101 \(2015\)](#)

Vibrational energy flow in the villin headpiece subdomain: Master equation simulations

David M. Leitner, Sebastian Buchenberg, Paul Brettel, Gerhard Stock
[J. Chem. Phys. 142, 075101 \(2015\)](#)

Theory and simulations of toroidal and rod-like structures in single-molecule DNA condensation

Ruggero Cortini, Bertrand R. Caré, Jean-Marc Victor, Maria Barbi
[J. Chem. Phys. 142, 105102 \(2015\)](#)

Dissipation enhanced vibrational sensing in an olfactory molecular switch

Agata Chęcińska, Felix A. Pollock, Libby Heaney, Ahsan Nazir
[J. Chem. Phys. 142, 025102 \(2015\)](#)

Effect of temperature on the low-frequency vibrational spectrum and relative structuring of hydration water around a single-stranded DNA

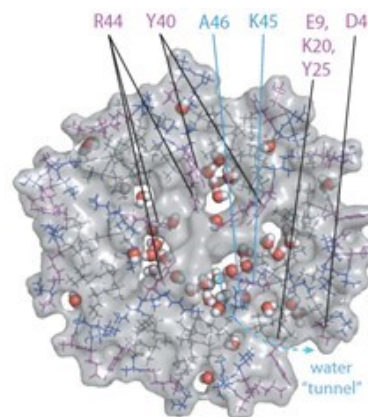
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Alexei Tkachenko and Sergei Maslov
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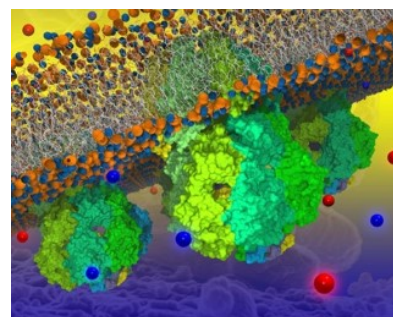
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Kaushik Chakraborty, Sanjoy Bandyopadhyay

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Dynamical role of phosphorylation on serine/threonine-proline Pin1 substrates from constant force molecular dynamics simulations

Hector A. Velazquez, Donald Hamelberg

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A comparative analysis of clustering algorithms: O₂ migration in truncated hemoglobin I from transition networks

Pierre-André Cazade, Wenwei Zheng, Diego Prada-Gracia, Ganna Berezovska, *et al.*

[J. Chem. Phys. 142, 025103 \(2015\)](#)

Investigation of the nanoviscosity effect of a G-quadruplex and single-strand DNA using fluorescence correlation spectroscopy

Dongkeun Lee, Minjung Kim, Soo Yong Kim, Hyosup Shin, *et al.*

[J. Chem. Phys. 142, 025101 \(2015\)](#)

Kinetic regulation mechanism of pbuE riboswitch

Sha Gong, Yujie Wang, Wenbing Zhang

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Asynchronous symmetry-based sequences for homonuclear dipolar recoupling in solid-state nuclear magnetic resonance

Kong Ooi Tan, M. Rajeswari, P. K. Madhu, Matthias Ernst

[J. Chem. Phys. 142, 065101 \(2015\)](#)

Which way up? Recognition of homologous DNA segments in parallel and antiparallel alignments

Dominic J. (O') Lee, Aaron Wynveen, Tim Albrecht, Alexei A. Kornyshev

[J. Chem. Phys. 142, 045101 \(2015\)](#)

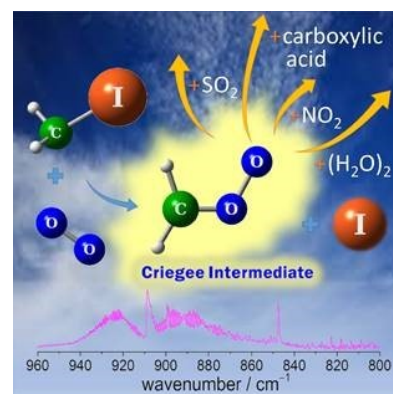
Flexibility of short DNA helices with finite-length effect: From base pairs to tens of base pairs

Yuan-Yan Wu, Lei Bao, Xi Zhang, Zhi-Jie Tan

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The effects of multiple probes on the hybridization of target DNA on surfaces

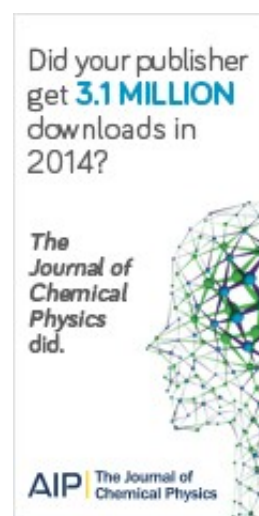
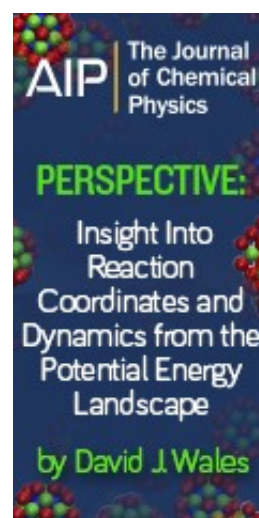
Ryan C. Welling, Thomas A. Knotts



Perspective: Spectroscopy and kinetics of small gaseous Criegee intermediates

Yuan-Pern Lee

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Increasing the sampling efficiency of protein conformational transition using velocity-scaling optimized hybrid explicit/implicit solvent REMD simulation

Yuqi Yu, Jinan Wang, Qiang Shao, Jiye Shi, *et al.*

[J. Chem. Phys. 142, 125105 \(2015\)](#)

Isotope-enriched protein standards for computational amide I spectroscopy

Mike Reppert, Anish R. Roy, Andrei Tokmakoff

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DNA-binding protein searches for its target: Non-monotonic dependence of the search time on the density of roadblocks bound on the DNA chain

Lin Liu, Kaifu Luo

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