Dr. Cecilia Clementi

CURRICULUM VITÆ ET STUDIORUM

Name : Cecilia Clementi
Nationality : USA, Italy (double citizenship)
Date of birth : November 9, 1971
Place of birth : Firenze, Italy
Languages : Italian (mother tongue), English (fluent)

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Positions:

2016–present	:	Einstein Visiting Fellow, Freie Universität Berlin, Germany
2013–present	:	Senior Investigator, Center for Theoretical Biological Physics, Rice University
2009–present	:	Full Professor, Rice University, Department of Chemistry
2008–present	:	Wiess Career Development Chair, Rice University, Department of Chemistry
2007–2009	:	Associate Professor (with tenure) at Rice University, Department of Chemistry
2006–present	:	Joint appointment in the Department of Chemical and Biomolecular Engineering, Rice University
2001–2007	:	Assistant Professor at Rice University, Department of Chemistry
2002–present	:	Faculty member of the *Structural and Computational Biology and Molecular Biophysics (SCBMB)* program, Baylor College of Medicine
2002–present	:	Faculty member of the *Keck Center for Computational Biology*, Rice University
2002–present	:	Faculty member of the *Applied Physics* program, Rice University
1998–2001	:	La Jolla Interfaces in Science (LJIS) Postdoctoral Fellow, at the University of California, San Diego, Department of Physics

Education:

October 1998	:	Ph.D. degree in Physics, full marks *cum laude*, International School for Advanced Studies (SISSA/ISAS), Trieste (Italy)
October 1996	:	M.Sc. degree in Physics, full marks *cum laude*, International School for Advanced Studies (SISSA/ISAS), Trieste (Italy)
March 1995	:	*Laurea* (B.S.) degree in Physics, full marks *cum laude*, University of Florence, Firenze (Italy)

Research Interests:

Data-driven Discovery of Physical Principles, *Statistical Mechanics*, *Multi-scale Physical Modeling*, *Biophysics*, *Macromolecular Simulation*

Honors and Awards:

- co-Director of NSF-funded Molecular Sciences Software Institute (MolSSI), 2016-present
- Einstein Visiting Fellowship, Einstein Foundation, Berlin, Germany, 2016-2019
- Hamill Innovation award, 2014
- Welch Foundation Norman Hackerman Award in Chemical Research, 2009
- Hamill Innovation award, 2007
- NSF-CAREER award, 2004–2009
- Norman Hackerman Welch Young Investigator award, 2001–2004
- La Jolla Interfaces in Science (LJIS) fellowship (supported by the Burroughs Wellcome Fund), 1999–2001
- SISSA research scholarship, 1995-1998

Research Grants:

Current:

- National Science Foundation ACI-1547580 “SI2I2: Impl: The Molecular Sciences Software Institute” - $20,269,420 (8 co-PIs, Dr. Daniel Crawford at Virginia Tech, Chemistry, is PI), 2016-2021
- National Science Foundation CHE-1738990 “D3SC: EAGER: Data-driven design of molecular models from microscopic dynamics and experimental data” - $300,000 (PI) 2017-2020
- Einstein Foundation (Berlin, Germany) “Bridging molecular and cellular resolution by multiscale modeling incorporating experimental data” - € 510,000 (PI) 2016-2019
- Welch Foundation C-1570 “Mapping the Free Energy Landscape of Proteins by Combining Theory and Experiment” - $330,000 (PI) 2016-2019
- National Science Foundation CHE-1265929 “Collaborative Research: S12-CHE: ExTASY Extensible Tools for Advanced Sampling and Analysis” - $686,115 (PI) 2013-2017
- National Science Foundation PHY-1427654 “Center for Theoretical Biological Physics – Houston” - $11,750,000 (14 co-PIs grant, Dr. Josè Onuchic at Rice University, Physics, is PI) 2014-2019
- National Science Foundation ACI-1331519 “Collaborative Research: S2I2: Conceptualization of a Center for Biomolecular Simulation” - $102,582 (3 co-PIs, Dr. Vijay Pande at Stanford, Chemistry, is PI) 2014-2017

Past:

- National Science Foundation ACI-1546678 “Designing and Assessing Effective Hands-On Training for Computational Science” - $12,000 (PI) 2015-2016
- Welch Foundation C-1570 "Mapping the Free Energy Landscape of Proteins by Combining Theory and Experiment" - $300,000 (PI) 2013-2016
- National Science Foundation CHE-1152344 “Multi-resolutions Framework for the Characterization of Protein Mechanisms” - $420,000 (PI) 2012-2016
- Welch Foundation C-1570 “Mapping the Free Energy Landscape of Proteins by Combining Theory and Experiment” - $200,000 (PI) 2011-2013
- National Science Foundation CHE-0835824 “CDI-Type I: A multidisciplinary, multiscale approach to discover organizing principles in macromolecular dynamics and functions” - $383,371 (PI) 2008-2011
- National Science Foundation CAREER CHE-0349303 “Holistic Approach to the Study of Protein Mechanisms” - $500,000 (PI) 2004-2009
- National Science Foundation CNS-0821727 “MRI: Acquisition of Cyberinfrastructure for Computational Research (CCR)” - $1,977,152 (5 co-PIs) 2008
- Welch Foundation C-1570 “Mapping the Free Energy Landscape of Proteins by Combining Theory and Experiment” - $150,000 (PI) 2007-2010
- National Science Foundation CCF-0523908 “A Computational Framework for the Characterization of Biological Systems at the Molecular Level” - $300,000 (2 co-PIs, Dr. Kavraki at Rice University, Computer Science, is PI) 2005-2008
- Texas Advanced Technology Program (Project # 003604-0010-2003) “Development of Geometric Tools for Computer-Aided Drug Discovery” - $200,000 (2 co-PIs, Dr. Kavraki at Rice University, Computer Science, is PI) 2004-2006
- National Science Foundation CNS-0454333 “CRI: Acquisition of Rice Physical and Biological Computing (PBC) Cluster” - $232,762 (co-PI, 5 PIs grant) 2005
- Welch Foundation C-1570 "Mapping the Free Energy Landscape of Proteins by Combining Theory and Experiment" - $150,000 (PI) 2004-2007
- The Welch Foundation (Norman Hackerman - Welch Young Investigator award) - $135,000 (PI) 2001-2004

Supercomputing Grants:

- 2017-2020 U.S. Department of Energy – INCITE Leadership Computing BIP149 “Unraveling autoimmune diseases with adaptive protein simulation”, 246 million core hours on Titan (Cray XK7) at Oak Ridge National Laboratories.
- 2017-2019 National Science Foundation – Petascale Computing Resource Allocations (PRAC) OAC-1713749 “More Power to the Many: Scalable Ensemble-based Simulations and Data Analysis”, 140 million core hours on Blue Waters (Cray XE6 and XK7) at the National Center for Supercomputing Applications, University of

Illinois.
- 2015-2016 National Science Foundation – Petascale Computing Resource Allocations (PRAC) OAC-1516469 "The Power of Many: Scalable Compute and Data-Intensive Science on Blue Waters", 24 million core hours on Blue Waters (Cray XE6 and XK7) at the National Center for Supercomputing Applications, University of Illinois.

Professional Service:

- Co-Director of NSF-funded Molecular Sciences Software Institute (MolSSI), 2016-present
- Organizer of IPAM semester-long program on "Complex High-Dimensional Energy Landscapes", 2017
- associated editor of J. Chem. Theory Comput., 2015–present
- UCLA Institute for Pure and Applied Mathematics (IPAM), Scientific Advisory Board Member, 2015-2018
- International Society of Quantum Biology and Pharmacology, Councilor, 2010-2013
- International Human Frontier Science Program (HFSP) Organization, Review Committee for Fellowships, 2008-2012
- Volkswagen Foundation, Scientific Board Panel Member, 2008-2010
- Chair of Biophysical Subdivision of the American Chemical Society (ACS) 2005-2008
- Organizer of IPAM semester-long program on "Bridging Time and Length Scales in Materials Science and Biophysics", 2015
- Reviewer for several scientific journals, including:
  Nature, Proc. Natl. Acad. Sci. USA, Phys. Rev. Lett., Phys. Rev. E, J. Am. Chem. Soc., J. Chem. Theory Comput., J. Chem. Phys., Biophys. J.
- Reviewer for NSF grant proposals evaluation (PHY, CHE, MCB, OAC)
- Reviewer for U.S. Army Research Office grant proposals evaluation

Selected Invited Presentations (180+ total):

- ☑ plenary talk presented at the "IUPAP XXIX Conference on Computational Physics", Paris, France, July 9-13 2017.
- ☑ invited talk presented at the *Annual Meeting of the American Physical Society*, New Orleans, LA, March 13-17, 2017
- ☑ invited talk presented at workshop on "*Collective Variables in Classical Mechanics*", Institute for Pure and Applied Mathematics (IPAM), UCLA, October 24-28 2016
- ☑ invited talk presented at the *National Meeting of the American Chemical Society*, San Diego, CA, March 13-17 2016.
- ☑ invited talk presented at the "*Molecular and Chemical Kinetics 2015*" conference Berlin, Germany, September 7-11 2015
- ☑ invited talk presented at the international symposium on "*Big Data and Predictive Computational Modeling*", Munich, Germany, May 18-21 2015.
- ☑ invited talk presented at the *National Meeting of the American Chemical Society*, Denver, CO, March 22-26, 2015
- ☑ invited talk presented at the workshop on "*Scale Bridging Techniques in Molecular Simulation: A Critical Appraisal*" in Berlin, Germany, August 25-27 2014
- ☑ invited talk presented at the *Gordon Conference on Computational Chemistry*, Mount Snow, VT, July 20-25 2014
- ☑ invited talk presented at the symposium on *"Physical Principles of Biomolecular Dynamics*", at USP, Sao Paulo, Brazil, May 23 2014
- ☑ invited talk presented at the *Berkeley Statistical Mechanics Meeting*, at UC Berkeley, CA, January 10-12 2014
- ☑ invited talk presented at the *National Meeting of the American Chemical Society*, Indianapolis, Indiana, September 8-12, 2013
- ☑ invited talk presented at the *"Molecular Kinetics"* meeting at Freie Universität Berlin, Germany, September 2-5 2013
- ☑ invited talk presented at the workshop on *"Physical Principles and Underlying Mechanisms of Biomolecules and Materials"* in Bejing, China, August 3-5 2013

- ☑ invited talk at the SIAM Conference on *"Mathematical Aspects of Materials Science"*, Philadelphia, June 9-12, 2013
- ☑ invited talk presented at the international workshop on *"Connecting Electrochemical and Water Simulations: Status and Future Challenges"*, Tegernsee, Germany, April 21-24 2013
- ☑ invited talk presented at *Annual Meeting of the American Physical Society*, Baltimore, MD, March 18-22 2013
- ☑ invited talk presented at the international conference on *"Biomolecular Dynamics: Computation Meets Experiment"*, at the King Abdullah University of Science and Technology (KAUST) in Saudi Arabia, February 22-25 2013
- ☑ invited talk presented at the *Annual Meeting of the Institute for Complex and Adaptive Matter (ICAM)*, New York City, May 23-26 2012
- ☑ distinguished lecture presented in the National Science Foundation *"Cyber-Enhanced Discovery and Innovation"* lecture series, Arlington, VA, September 1, 2011
- ☑ invited talk presented at the workshop on *"Expanding the Frontiers of Biomolecular Science"*, Juelich, Germany, November 15-17, 2010
- ☑ invited talk presented at the *National Meeting of the American Chemical Society*, San Francisco, CA, March 21-25, 2010
- ☑ invited talk presented at the *VolkswagenStiftung symposium "Computer Simulation of Molecular and Cellular Biosystems and Complex Soft Matter"*, Mainz, Germany, September 20-24, 2009
- ☑ invited talk presented at the *"Femtophysics - Frontiers in Ultrafast Science and Technology (Femtochemistry IX)"*, Beijing, China, August 8-13, 2009
- ☑ invited talk presented at the *Annual Meeting of the American Physical Society*, Pittsburgh, PA, March 16-20, 2009
- ☑ invited talk presented at the *Annual Meeting of the Biophysical Society*, workshop on *"Protein Folding and Stability"*, Boston, MA, March 1-5, 2009
- ☑ invited talk presented at the *National Meeting of the American Chemical Society*, Philadelphia, PA, August 17-21, 2008
- ☑ invited talk presented at the international workshop on *"Multiscale methods for the design of biofunctional molecules"*, University of Duisburg-Essen, Germany, April 2-5, 2008.
- ☑ three invited lectures presented at the ICAM/FAPERJ school on *"Biological Physics at the Molecular/Cellular Interface"*, Rio de Janeiro, Brazil, March 16-23, 2008.
- ☑ invited talk presented at the *Gordon Research Conference on "Protein Folding Dynamics"*, Ventura, CA, January 6-11, 2008.
- ☑ invited talk presented at the IUPAP international conference on *"Biological Physics"*, Montevideo, Uruguay, August 27-31, 2007
- ☑ invited talk presented at the international meeting on *"Theory and Simulation of Biomolecular Nano-Machines"*, Kobe, Japan, December 12-16, 2006
- ☑ invited talk presented at the *WE-Heraeus-Seminar on "Biomolecular Simulation: From Physical Principles to Biological Function"*, Bad Honnef, May 22–24, 2006
- ☑ invited talk presented at the *"US-Japan symposium on Protein Folding and Design"*, Philadelphia, PA, May 2–5, 2005
- ☑ invited talk presented at the National Science Foundation workshop on *"Molecular Basis of Life Processes"*, Oak Ridge National Laboratory (ORNL), Oak Ridge, TN, October 28–30, 2004
- ☑ plenary lecture presented at the *"18th Molecular Modeling Workshop"*, Computer-Chemie-Centrum, Erlangen (Germany) May 18–19, 2004
- ☑ invited talk presented at the *Gordon Research Conference on "Protein Folding Dynamics"*, Ventura, CA, January 11-16, 2004.
- ☑ invited talk presented at the *National Meeting of the American Chemical Society* , New Orleans, LA, March 23–27, 2003
- ☑ invited talk presented at the *Annual Meeting of the American Physical Society*, Indianapolis, Indiana, March 18–22 2002

Book Chapters:

1. *"Coarse Graining Models for Protein Folding"* S. Matysiak, C. Clementi
   Book chapter in "Coarse-graining in Condensed Phase and Biomolecular Systems",
   ed. G.Voth, (Taylor and Francis, 2008)

Papers on Refereed Journals :

h-index 33, 4380+ citations (August 2017)

1. *"Learning effective molecular models from global observables"*
   J. Chen, J. Chen, C. Clementi
   J. Am. Chem. Soc., submitted (2017)
2. *"A data-driven perspective on the hierarchical assembly of molecular structures"*
   L. Boninsegna, R. Banisch, C. Clementi
   Proc. Natl. Acad. Sci. USA, submitted (2017)
3. *"On the origin of phase transitions in the absence of symmetry-breaking"*
   G. Pettini, M. Gori, R. Franzosi, C. Clementi, M. Pettini
   Phys. Rev. E, submitted, arXiv:1706.07950 (2017)
4. *"Combining experimental and simulation data of molecular processes via augmented Markov models"*
   S. Olsson, H. Wu, F. Paul, C. Clementi, and F. Noé
   Proc. Natl. Acad. Sci. USA, (2017) in press (published online August 2017) DOI: 10.1073/pnas.1704803114
5. *"Collective variables for the study of long-time kinetics from molecular trajectories: theory and methods"*
   F. Noé, C. Clementi
   Curr. Opin. Struct. Biol. 43, 141-147 (2017)
6. *"Path integral-GC-AdResS simulation of a large hydrophobic solute in water: a tool to investigate the interplay between local microscopic structures and quantum delocalization of atoms in space"*
   A. Agarwal, C. Clementi, L. Delle Site
   Phys. Chem. Chem. Phys. 19 (20), 13030-13037 (2017)
7. *"Markov State Models from short non-Equilibrium Simulations-Analysis and Correction of Estimation Bias"*
   F. Nüske, H. Wu, J.-H. Prinz, C. Clementi, F. Noé
   J. Chem. Phys. 146, 094104 (2017)
8. *"Commute maps: separating slowly-mixing molecular configurations for kinetic modeling"*
   F Noé, R Banisch, C. Clementi
   J. Chem. Theory Comput., 12 (11), 5620-5630 (2016)
9. *"ExTASY: Scalable and Flexible Coupling of MD Simulations and Advanced Sampling Techniques"*
   V. Balasubramanian, I. Bethune, A. Shkurti, E. Breitmoser, E. Hruska, C. Clementi, C. Laughton, S. Jha
   2016 IEEE 12th International Conference on e-Science (e-Science) in press (2016)
10. *"Investigating Molecular Kinetics by Variationally Optimized Diffusion Maps"*
    L. Boninsegna, G. Gobbo, F. Noé, C. Clementi
    J. Chem. Theory Comput., 11 (12), 5947-5960 (2015)
11. *"Kinetic distance and kinetic maps from molecular dynamics simulation"*
    F. Noé, C. Clementi
    J. Chem. Theory Comput. 11 (10), 5002-5011 (2015)
12. *"Operating principles of Notch-Delta-Jagged module of cell-cell communication"*
    M.K. Jolly, M. Boareto, M, Liu, J.N. Onuchic, C. Clementi, E. Ben-Jacob
    New J. Phys. 17 055021 (2015)
13. *"Jagged-Delta asymmetry in Notch signaling can give rise to a Sender/Receiver hybrid phenotype"*
    M. Boareto, M.K. Jolly, M. Liu, J.N. Onuchic, C. Clementi, E. Ben-Jacob
    Proc. Natl. Acad. Sci. USA 112, E402-E409 (2015)
14. *"A comparative analysis of clustering algorithms: O-2 migration in truncated hemoglobin I from transition networks"*
    P.A. Cazade, W. Zheng, D. Prada-Gracia, G. Berezovska, F. Rao, C. Clementi, M. Meuwly
    J. Chem. Phys. 142 025103 (2015)
15. *"Multiscale approach to the determination of the photoactive yellow protein signaling state ensemble"*

M.A. Rohrdanz, W. Zheng, B.P. Lambeth, J. Vreede, C. Clementi
Plos Comp. Biol. 10 e1003797 (2014)

16. *"Fast Recovery of Free Energy Landscapes via Diffusion-Map-directed Molecular Dynamics"*
J. Preto, C. Clementi
Phys. Chem. Chem. Phys. 16 19181-19191 (2014)
17. *"A tripodal monopeptide ligand for asymmetric Rh(II) catalysis and the importance of on-bead catalyst development"*
R. Sambasivan, W. Zheng, S.J. Burya, B.V. Popp, C. Turro, C. Clementi, Z.T. Ball
Chem. Sci. 5 1401 (2014)
18. *"Molecular recognition of DNA by ligands: Roughness and complexity of the free energy profile"*
W. Zheng, A.V. Vargiu, M.A. Rohrdanz, P. Carloni, C. Clementi
J. Chem. Phys. 139 145102 (2013)
19. *"Rapid Exploration of Configuration Space with Diffusion-Map-Directed Molecular Dynamics"*
W. Zheng, M.A. Rohrdanz, C. Clementi,
J. Phys. Chem. B 42 12769-12776 (2013)
20. *"Discovering mountain passes via torchlight: methods for the definition of reaction coordinates and pathways in complex macromolecular reactions"*
M.A. Rohrdanz, W. Zheng, C. Clementi
Ann. Rev. Phys. Chem. 64 295-316 (2013)
21. *"AWSEM-MD: Protein structure prediction using coarse-grained physical potentials and bioinformatically based local structure biasing"*
A. Davtyan, N.P. Schafer, W. Zheng, C. Clementi, P.G. Wolynes, G.A. Papoian
J.Phys. Chem. B 116, 8494-8503 (2012)
22. *"Delineation of folding pathways of a beta-sheet miniprotein"*
W. Zheng, B. Qi, M.A. Rohrdanz, A. Caflisch, A.R. Dinner, C. Clementi
J. Phys. Chem. B 115, 13065-13074 (2011)
23. *"A new perspective on transition states: χ_1 separatrix"*
P.J. Ledbetter, C. Clementi
J. Chem. Phys. 135, 044116 (2011)
24. *"Polymer reversal rate calculated via locally scaled diffusion map"*
W. Zheng, M.A. Rohrdanz, M. Maggioni, C. Clementi
J. Chem. Phys. 134, 144108 (2011)
25. *"Determination of reaction coordinates via locally scaled diffusion map"*
M.A. Rohrdanz, W. Zheng, M. Maggioni, C. Clementi
J. Chem. Phys. 134, 124116 (2011)
26. *"Reconstruction of folding free energy landscape using an equation-free approach"*
P. Das, T.A. Frewen, I.G. Kevrekidis, C. Clementi
Lecture Notes in Computational Science and Engineering, 75, 113-131 (2011)
27. *"Communication: On the locality of hydrogen bond networks at hydrophobic interfaces"*
B.P. Lambeth, C. Junghans, K. Kremer, C. Clementi, L. Delle Site,
J. Chem. Phys., 133, 221101 (2010) (cover article)
28. *"Application of Non-Linear Dimensionality Reduction to Characterize the Conformational Landscape of Small Peptides"* H. Stamati, L.E. Kavraki, C. Clementi
Proteins: Structure, Function and Bioinformatics, 78, 223-235 (2010)
29. *"Restriction vs. Guidance: Fragment Assembly and Associative Memory Hamiltonians for Protein Structure Prediction"*
J.A. Hegler, J. Latzer, A. Shehu, C. Clementi, P.G. Wolynes
Proc. Natl. Acad. Sci. USA, 106, 15302-15307 (2009)
30. *"Multiscale Characterization of Protein Conformational Ensembles"* A. Shehu, L.E. Kavraki, C. Clementi
Proteins: Structure, Function and Bioinformatics, 76, 837-851 (2009)
31. *"Coarse-Grained Models of Protein Folding"*
C. Clementi

Curr. Opin. Struct. Biol. 18, 10-15, (2008)

32. *"Mapping Folding Energy Landscapes with Theory and Experiment"*
S. Matysiak, C. Clementi
Arc. Biochem. Biophys. 469, 29-33 (2008)
33. *"Unfolding the Fold of Cyclic Cysteine-rich Peptides"*
A. Shehu, L.E. Kavraki, C. Clementi
Protein Science 17, 482-493 (2008)
34. *"Modeling diffusive dynamics in adaptive resolution simulation of liquid water"*
S. Matysiak, C. Clementi, M. Praprotnik, K. Kremer, L. delle Site
J. Chem. Phys. 128, 024503 (2008)
35. *"Adaptive resolution simulation of liquid water"*
M. Praprotnik, S. Matysiak, L. Delle Site, K. Kremer, C. Clementi
J. Phys.: Condens. Matter 19, 292201 (2007)
36. *"From coarse-grain to all-atom: Toward multiscale analysis of protein landscapes"*
A.P. Heath, L.E. Kavraki, C. Clementi
Proteins: Structure, Function and Bioinformatics 68, 646-661 (2007) (cover article)
37. *"Fast and reliable analysis of molecular motion using proximity relations and dimensionality reduction"*
E. Plaku, H. Stamati, C. Clementi, L.E. Kavraki
Proteins: Structure, Function and Bioinformatics 67, 897-907 (2007)
38. *"On the characterization of protein native state ensembles"*
A. Shehu, L.E. Kavraki, C. Clementi
Biophysical Journal 92, 1503-1511 (2007)
39. *"Supersymmetric Langevin equation to explore free energy landscapes"*
A. Mossa, C. Clementi
Phys. Rev. E 75, 046707 (2007)
40. *"Sampling conformation space to model equilibrium fluctuations in proteins"*
A. Shehu, C. Clementi, L.E. Kavraki
Algorithmica 48, 303-327 (2007)
41. *"Minimalist protein model as a diagnostic tool for misfolding and aggregation"*
S. Matysiak, C. Clementi
J. Mol. Biol. 363, 297-308 (2006)
42. *"Hamiltonian dynamics of homopolymer chain models"*
A. Mossa, M. Pettini, C. Clementi
Phys. Rev. E 74, 041805 (2006)
43. *"Modeling protein conformational ensembles: From missing loops to equilibrium fluctuations"*
A. Shehu, C. Clementi, L.E. Kavraki
Proteins: Structure, Function and Bioinformatics 65, 164-179 (2006)
44. *"Low-dimensional free energy landscapes of protein folding reactions by nonlinear dimensionality reduction"*
P. Das, M. Moll, H. Stamati, L.E. Kavraki, C. Clementi
Proc. Natl. Acad. Sci. USA 103, 9885-9890 (2006)
45. *"Dynamics of polymer translocation through a nanopore: Theory meets experiment"*
S. Matysiak, A. Montesi, A.B. Kolomeinsky, M. Pasquali, C. Clementi
Phys. Rev. Lett. 96, 118103 (2006)
46. *"Characterization of the folding landscape of monomeric lactose repressor: Quantitative comparison of theory and experiment"*
P. Das, C.J. Wilson, G. Fossati, P. Wittung-Stafshede, K.S. Matthews, C. Clementi
Proc. Natl. Acad. Sci. USA 102, 14569-14574 (2005)
47. *"The experimental folding landscape of monomeric lactose repressor, a large two-domain protein, involves two kinetic intermediates"*
C.J. Wilson, P. Das, C. Clementi, K.S. Matthews, P. Wittung-Stafshede
Proc. Natl. Acad. Sci. USA 102, 14563-14568 (2005)
48. *"Balancing energy and entropy: A minimalist model for the characterization of protein folding landscapes"*

P. Das, S. Matysiak, C. Clementi
Proc. Natl. Acad. Sci. USA 102, 10141-10146 (2005)

49. *"Optimal combination of theory and experiments for the characterization of the protein folding landscape of S6: how far can a minimalist model go?"*
S. Matysiak, C. Clementi
J. Mol. Biol. 343, 235-248 (2004)
50. *"Effect of non-native interactions on protein folding rate and mechanism"*
C. Clementi, S.S. Plotkin
Protein Science 13:7, 1750-1766 (2004)
51. *"Quantifying the roughness on the free energy landscape: Entropic bottlenecks and protein folding rates*
L.C. Chavez, J.N. Onuchic,C. Clementi
J. Am. Chem. Soc. 126:27, 8426-8432 (2004)
52. *"Interplay among tertiary contacts, secondary structure formation and side-chain packing in the protein folding mechanism: an all-atom representation study"*
C. Clementi, A.E. Garcia, J.N. Onuchic
J. Mol. Biol. 326, 933-954 (2003)
53. *"A geometric interpretation of integrable motions"*
C. Clementi, M. Pettini
Celest. Mech. & Dyn. Astr. 84, 263-281 (2002)
54. *"Prediction of folding mechanism for circular–permuted proteins"*
C. Clementi, P.A. Jennings, J.N. Onuchic
J. Mol. Biol. 311, 879-890 (2001)
55. *"How native state topology affects the folding of Dihydrofolate Reductase and Interleukin-1β"*,
C. Clementi, P.A. Jennings, J.N. Onuchic
Proc. Natl. Acad. Sci. USA 97, 5871-5876 (2000)
56. *"Topological and energetic factors: what determines the structural details of the transition state ensemble and "on–route" intermediates for protein folding? An investigation for small globular proteins"*,
C. Clementi, H. Nymeyer, J.N. Onuchic,
J. Mol. Biol. 298, 937-953 (2000)
57. *"Hamiltonian dynamics and geometry of phase transitions in XY models"*,
M. Cerruti–Sola, C. Clementi, M. Pettini,
Phys. Rev. E 61, 5171-5190 (2000)
58. *"Folding Lennard–Jones proteins by a contact potential"*,
C. Clementi, M. Vendruscolo, A. Maritan, E. Domany,
Proteins: Structure, Function and Genetics, 97, 544 (1999)
59. *"Protein design is a key factor for subunit-subunit association"*,
C. Clementi, P. Carloni, A. Maritan,
Proc. Natl. Acad. Sci. USA 96, 9616 (1999)
60. *"Determination of interaction potentials of amino acids from native protein structures: Tests on simple lattice models"*,
J.van Mourik, C. Clementi, F. Seno, A. Maritan, J.R. Banavar,
J. Chem. Phys. 110, 10123 (1999)
61. *"Folding, design and determination of interaction potentials using off-lattice dynamics of model heteropolymers"*,
C. Clementi, A. Maritan, J.R. Banavar,
Phys. Rev. Lett. 81, 3287 (1998)
62. *"Geometry of dynamics and phase transitions in classical lattice ϕ^4 theories"*,
L. Casetti, L. Caiani, C. Clementi, M. Pettini, G. Pettini, R. Gatto,
Phys. Rev. E 57, 3886 (1998)
63. *"Geometry of dynamics, Lyapunov exponents and phase transitions"*,
L. Casetti, L. Caiani, C. Clementi, M. Pettini,

Phys. Rev. Lett. 79, 4361 (1997)
64. *"Riemannian theory of Hamiltonian chaos and Lyapunov exponents"*,
L. Casetti, C. Clementi, M. Pettini,
Phys. Rev. E 54, 5969 (1996)