Alberto Perez

Contact Information

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Research Interests

Protein-protein, protein-peptide and protein-DNA interactions, molecular recognition, drug design, structure prediction and dynamics.

Publication Summary

Google scholar statistics: `https://goo.gl/WHhPMX`
Total papers: 49, *Total citations:* 4200, *H-index:* 28

Education

Doctor of Philosophy, Physical Chemistry 2003-2008
-Advisors: Modesto Orozco, F. Javier Luque
-University of Barcelona
-Developed better physical models for DNA and developed told to characterize sequence dependent properties of DNA.
-Dissertation title: Macromolecular Interactions

Bachelor of Science, Chemistry 1998-2002
-University of Barcelona

Research Experience

Assistant Professor 2018-present
-Chemistry Department , University of Florida

Research Assistant Professor 2014-2018
-Laufer Center for Physical and quantitative Biology, Stony Brook University
-Use of general knowledge for protein structure prediction and peptide protein binding.

Laufer Junior fellow 2013-2018
-Laufer Center for Physical and Quantitative Biology, Stony Brook University
-Developed integrative tools for protein structure prediction and recognition.

Postdoctoral Fellow 2010-2013
-Advisor: Ken Dill
-University of California San Francisco and Stony Brook University
-Developed integrative tools for protein structure prediction and recognition.

Postdoctoral Fellow 2009-2010
-Advisors: Modesto Orozco
-Barcelona Supercomputing Center
-Linked atomistic physical properties of DNA to genomic functionality.

Fellowships

-European Molecular Biology Organization (EMBO) (**$85K** total) 2010-2012
-Juan de la Cierva Postdoctoral fellowship (**€33.6K/year**) 2009-2010
-Short term visiting scientist (U. of Minnesota) fellowship (Catalan government) 2005
-Catalan fellowship towards PhD studies (**€44K total**) 2004-2007
-University of Barcelona fellowship towards PhD studies (declined) 2004
-University of Barcelona fellowship for internship research 2002-2003

Research Grants

-NIH: (2017) Helped write NIH R01, funded for **$2m** over 5 years. PI: Ken A. Dill
-NSF: (2017) Petascale Computing Resource Allocation: **$15.6K travel award + 11.3 million node hours** of computing at Blue Waters Supercomputer. PIs: Ken A. Dill, Alberto Perez.
-NSF: (2015) Petascale Computing Resource Allocation: **$30K travel award + 7 million node hours** of computing at Blue Waters Supercomputer. PIs: Ken A. Dill, Alberto Perez.
-NIH: (2013) Helped write NIH R01, funded for **$2m** over 5 years. PIs: Carlos Simmerling, Ken A. Dill
-XSEDE: (2013) Awarded 500k hours on Keeneland. PIs: J.L. MacCallum and A. Perez.
-ALCC (2012): Awarded 2000k hour leadership class allocation on Titan. PI: K.A. Dill
-XSEDE (2011): Awarded 750k hours on GPU enabled Forge and Keeneland clusters. PIs: J.L. MacCallum and A. Perez

Teaching Experience

University of Florida
Chemical Bond and Spectra (graduate level, CHM 6470) Fall 2018
Stony Brook University
Physical and Quantitative Biology (invited lecturer) 2015
Barcelona Supercomputing Center
Getting the most from biomolecular simulations: a practical workshop 2008
University of Barcelona
General Chemistry (Biology Dept., 240 hours, Freshman Biology students) 2007-2008
Bioinformatics (Master in Biomedicine) 2006-2007
Physicochemistry (Pharmacy Dept., sophomore students) 2005-2006
Molecular Dynamics (Postgraduate course) 2004-2005
Clinical Biochemistry (Biology Dept., senior students) 2002-2003
General Chemistry (Biology Dept., Freshman Biology students) 2002-2003

Presentations

Scientific Conferences and invited talks
-FAME (Florida ACS sub-meeting), Tampa Bay, Florida (talk) 2019
-National ACS meeting, Orlando, Florida (talk) 2019
-59th Sanibel Symposium, St. Simons Island, Georgia (poster) 2019
-CASP13, Cancun, Mexico (talk) 2018
-Statistical Physics in Biology (Honor of Ken Dill Symposium), Phoenix, Arizona (talk) 2018
-Blue Waters Symposium, Sunriver, Oregon (talk) 2018
-101st Canadian Chemistry Conference, Edmonton (talk) 2018
-Chemistry Department, University of Florida (talk) 2018
-Okinawa Institute of Science and Technology, Japan (talk) 2018
-Protein and RNA Structure Prediction, Jamaica (talk) 2017
-American Chemical Society, San Francisco (talk) 2017
-Blue Waters Symposium, Sunriver, Oregon (poster) 2017
-Understanding Biology Through Structure Symposium, Santa Fe (poster) 2017

-Department of Chemistry, University of Utah (talk)	2017
-Department of Molecular Biosciences, University of Kansas (talk)	2017
-Chemistry Department, Lehman College (talk)	2017
-School of Molecular Sciences, Arizona State University (talk)	2017
-Telluride workshop on Coarse-Grained Modeling, Telluride (talk)	2016
-Blue Waters Symposium, Sunriver, Oregon (talk)	2016
-Biophysical Society 60th meeting, Los Angeles (talk)	2016
-Graduate Center, College University of New York, (talk)	2016
-Chemistry Department, NorthEastern University, Boston, (talk)	2016
-Rules of Protein-DNA Recognition. Oaxaca, Mexico (talk)	2015
-New York Theoretical and Computational Chemistry Conference, (talk)	2015
-Biodesign meeting at Rutgers University in Piscataway, NJ. (talk)	2015
-Biophysical Society 59th meeting, Baltimore (poster)	2015
-Chemistry Department, Oklahoma University (talk)	2014
-CASP11: predictors meeting, Mexico (poster)	2014
-Zing: protein folding, Punta Cana (talk)	2014
-ISQBP meeting, Telluride (talk)	2014
-Biophysical society 58th meeting, San Francisco (talk)	2014
-Zing: Protein and RNA Structure Prediction, Playa del Carmen (talk)	2013
-Albany Conversations, Albany (talk)	2013
-Biophysical Society 57th Meeting, Philadelphia (poster)	2013
-CASP10: predictors meeting, Italy (poster)	2014
-Weslayan University Seminar Series (talk)	2012
-EMBO Fellows meeting (talk)	2012
-Rutgers Physics Department (talk)	2011
-CECAM workshop: Coarse-Grain Mechanics of DNA (talk)	2011
-UCSF: Andrej Sali's lab (talk)	2009
-DNA symposium (RANN VI) (talk)	2007
-DNA symposium (RANN V) (talk)	2005
-DNA symposium (RANN IV) (talk)	2003

General audience

-Brookhaven National Lab summer camp: Proteins in motion	2014
-World of physics(SBU): Proteins? Yes, please! (but folded)	2014
-TEDxSBU: You can't always blame your parents	2013
-Brookhaven National Lab summer camp: Proteins in motion	2013
-Sachem Library: Untangling DNA	2013
-Patchogue-Medford High school career day	2013
-Stony Brook Postdoc Symposium: Proteins?Yes, please (but folded)	2012

Oganized Conferences/Subsections

- Chair Computation Chemistry Symposium in FAME. Tampa Bay, FL 2019

Service

-Reviewer for the RES (Spanish supercomputing net, equivalent to XSEDE) since 2013.
-Judge at Brookhaven National Lab for Elementary school science fair.
-Panelist for DOE at Brookhaven National Lab *Life as a postdoc*. 2012 DOE SCGF Annual research meeting.
-**Peer review:** Journal of Chemical Theory and Computation, Nucleic acids research, Journal of the American Chemical Society, PLOS computational Biology, Briefings in Functional Genomics, Journal of Biomolecular Structure and Dynamics, BBA -

Proteins and Proteomics, PLOS One, Physical Chemistry Chemical Physics, WIREs Computational Molecular Science, The Journal of Physical Chemistry, Bioinformatics

Leadership

-Co-organizer of the Postdoc Symposium at Stony Brook (2012-2013).
-Founding member of the Stony Brook University Postdoctoral Association.
-Initial member of the Science Unplugged program at Stony Brook for science communication.

Affiliations

-Biophysical Society Member
-New York Academy of Sciences
-Faculty of 1000
-EMBO network

Publications

Refereed Research Papers

1. Perez, A., Gaalswyk, K., Jaroniec, C. P., and MacCallum, J. L. High Accuracy Protein Structures from Minimal Sparse Paramagnetic Solid-State NMR Restraints. *Angewandte Chemie*, 58(20), 6564?6568. (2019).
2. Ignatov, M., Liu, C., Alekseenko, A., Sun, Z., Padhorny, D., Kotelnikov, S., et al. . Monte Carlo on the manifold and MD refinement for binding pose prediction of protein-ligand complexes: 2017 D3R Grand Challenge. *Journal of Computer-Aided Molecular Design*, 33(1), 119?127.(2019)
3. Robertson, J. C., Perez, A., and Dill, K. MELD x MD Folds Nonthreadables, Giving Native Structures and Populations. *J Chem Theory Comput*, 14(12), 6734?6740. (2018)
4. Balaceanu, A., Perez, A., Dans, P. D., and Orozco, M. (2018). Allosterism and signal transfer in DNA. Nucleic Acids Research, 308(15), 1424?7565.
5. Perez, Alberto; Sittel, Florian; Stock, Gerhard and Dill, Ken. Protein conformational changes can take broad ensembles of routes. *J Chem Theory Comput* 14, 2109–2116 (2018).
6. Li, J., Sagendorf, JM., Chiu, TP., Pasi, M., Perez, A., and Rohs, R. Expanding the repertoire of DNA shape features for genome-scale studies of transcription factor binding. *Nucleic Acids Res.* (2017). 45 (22), 12877-12887
7. Sahu, S. et al. Regulation of the activity of the promoter of RNA-induced silencing, C3PO. *Protein Science* 20, 90 (2017).
8. Perez, A., Morrone, J. A., and Dill, K. (2017). Accelerating physical simulations of proteins by leveraging external knowledge. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, 125(Database issue), e1309.
9. Morrone, J. A. et al. Molecular Simulations Identify Binding Poses and Approximate Affinities of Stapled α-Helical Peptides to MDM2 and MDMX. *J Chem Theory Comput* 13, 863-869 (2017).
10. Morrone, J. A., Perez, A., MacCallum, J. and Dill, K. Computed Binding of Peptides to Proteins with MELD-Accelerated Molecular Dynamics. *J Chem Theory Comput* 13, 870-876 (2017).
11. Perez, A., Morrone, J. A., Brini, E., MacCallum, J. L. and Dill, K. A. Blind protein structure prediction using accelerated free-energy simulations. *Science Advances* 2 (11), e1601274-e1601274 (2016).
12. Perez, A., Morrone, J.A., Simmerling, C., Dill, K.A. Advances in free-energy simulations of protein folding and ligand binding. *Curr. Opin. Struct. Biol.* 36, 25-31 (2016)

13. I. Ivani, et. al. Parmbsc1: A refined force-field for DNA simulations. *Nature Methods*, 13, 55-58 (2016)

14. Perez, A., MacCallum, J.L., Coutsias, E.A., Dill, K.A. Constraint methods that accelerate free-energy simulations of biomolecules. *J. Chem. Phys.* 143, 243143 (2015)

15. Perez, A., MacCallum, J.L., Brini, E., Simmerling, C. and Dill, K.A. A grid-based backbone correction to the ff12SB protein force field for implicit-solvent simulations" *J Chem Theory Comput* 11, 4770-4779 (2015)

16. Perez, A.*, MacCallum, J. L.* and Dill, K. Accelerating molecular simulations of proteins using Bayesian inference on weak information. *Proc. Natl. Acad. Sci. U.S.A.* 112, 11846-11851 (2015)

17. Toledo, A., Perez, A., Coleman, J. L. and Benach, J. L. The lipid raft proteome of Borrelia burgdorferi. *Proteomics* 15, 3662-3675 (2015)

18. Nguyen, H., Perez, A., Bermeo, S. and Simmerling, C. Refinement of Generalized Born Implicit Solvation Parameters for Nucleic Acids and Their Complexes with Proteins. *J Chem Theory Comput* 11, 3714-3728 (2015).

19. J.L MacCallum*, A. Perez*, K.A. Dill, Determining protein structures by combining semireliable data with atomistic physical models by Bayesian inference (2015) *Proc. Natl. Acad. Sci. U.S.A.* 112, 6985-6990 (2015). * indicates equal contribution

20. Pasi, M. et al. μABC: a systematic microsecond molecular dynamics study of tetranucleotide sequence effects in B-DNA. *Nucleic Acid Research* 42, 12272-12283 (2014).

21. Perez, A. et al. Extracting representative structures from protein conformational ensembles. *Proteins: structure, function and bioinformatics* 82, 2671-2680 (2014).

22. Roy, A., Perez, A., Dill, K. A. and MacCallum, J. L. Computing the Relative Stabilities and the Per Residue Components in Protein Conformational Changes. *Structure* 22, 168-175 (2013).

23. Candotti, M. et al. Exploring early stages of the chemical unfolding of proteins at the proteome scale. *PLoS Comput. Biol.* 9, e1003393 (2013).

24. Drsata, T. et al. Structure, Stiffness and Substates of the Dickerson-Drew Dodecamer. *J Chem Theory Comput* 9, 707-721 (2013).

25. Dans, P. D., Perez, A., Faustino, I., Lavery, R. and Orozco, M. Exploring polymorphisms in B-DNA helical conformations. *Nucleic Acids Res.* 40, 10668-10678 (2012).

26. Perez, A. et al. Impact of methylation on the physical properties of DNA. *Biophys. J.* 102, 2140-2148 (2012).

27. Perez, A., Luque, F. J. and Orozco, M. Frontiers in molecular dynamics simulations of DNA. *Acc. Chem. Res.* 45, 196-205 (2012).

28. Perez, A., Yang, Z., Bahar, I. and Dill, K. A. FlexE: using elastic network models to compare models of protein structure. *J Chem Theory Comput* 8, 3985-3991 (2012).

29. Deniz, O. et al. Physical properties of naked DNA influence nucleosome positioning and correlate with transcription start and termination sites in yeast. *BMC Genomics* 12, 489 (2011).

30. MacCallum, J. L. et al. Assessment of protein structure refinement in CASP9. *Proteins* 79 Suppl 10, 74-90 (2011).

31. Meyer, T. et al. MoDEL (Molecular Dynamics Extended Library): a database of atomistic molecular dynamics trajectories. *Structure* 18, 1399-1409 (2010).
32. Faustino, I., Perez, A. and Orozco, M. Toward a consensus view of duplex RNA flexibility. *Biophys. J.* 99, 1876-1885 (2010).
33. Perez, A. and Orozco, M. Real-time atomistic description of DNA unfolding. *Angew. Chem. Int. Ed. Engl.* 49, 4805-4808 (2010).
34. Lavery, R. et al. A systematic molecular dynamics study of nearest-neighbor effects on base pair and base pair step conformations and fluctuations in B-DNA. *Nucleic Acids Res.* 38, 299-313 (2010).
35. Goni, J. R., Fenollosa, C., Perez, A., Torrents, D. and Orozco, M. DNAlive: a tool for the physical analysis of DNA at the genomic scale. *Bioinformatics* 24, 1731-1732 (2008).
36. Svozil, D. et al. Geometrical and electronic structure variability of the sugar-phosphate backbone in nucleic acids. *J Phys Chem B* 112, 8188-8197 (2008).
37. Gros, J. et al. 8-Amino guanine accelerates tetramolecular G-quadruplex formation. *Chem. Commun.* (Camb.) 2926-2928 (2008). doi:10.1039/b801221k
38. Orozco, M., Noy, A. and Perez, A. Recent advances in the study of nucleic acid flexibility by molecular dynamics. *Curr. Opin. Struct. Biol.* 18, 185-193 (2008).
39. Perez, A., Lankas, F., Luque, F. J. and Orozco, M. Towards a molecular dynamics consensus view of B-DNA flexibility. *Nucleic Acids Res.* 36, 2379-2394 (2008).
40. Perez, A., Luque, F. J. and Orozco, M. Dynamics of B-DNA on the microsecond time scale. *J. Am. Chem. Soc.* 129, 14739-14745 (2007).
41. Perez, A. et al. Refinement of the AMBER force field for nucleic acids: improving the description of alpha/gamma conformers. *Biophys. J.* 92, 3817-3829 (2007).
42. Rueda, M. et al. A consensus view of protein dynamics. *Proc. Natl. Acad. Sci. U.S.A.* 104, 796-801 (2007).
43. Goni, J. R., Perez, A., Torrents, D. and Orozco, M. Determining promoter location based on DNA structure first-principles calculations. *Genome Biol.* 8, R263 (2007).
44. Noy, A., Perez, A., Laughton, C. A. and Orozco, M. Theoretical study of large conformational transitions in DNA: the BA conformational change in water and ethanol/water. *Nucleic Acids Res.* 35, 3330-3338 (2007).
45. Meyer, T. et al. Essential Dynamics: A Tool for Efficient Trajectory Compression and Management. *J Chem Theory Comput* 2, 251-258 (2006).
46. Noy, A. et al. Data mining of molecular dynamics trajectories of nucleic acids. *J. Biomol. Struct. Dyn.* 23, 447-456 (2006).
47. Perez, A. et al. Exploring the Essential Dynamics of B-DNA. *J Chem Theory Comput* 1, 790-800 (2005).
48. Perez, A. et al. Are the hydrogen bonds of RNA (AU) stronger than those of DNA (AT)? A quantum mechanics study. *Chemistry* 11, 5062-5066 (2005).
49. Noy, A., Perez, A., Marquez, M., Luque, F. J. and Orozco, M. Structure, recognition properties, and flexibility of the DNA.RNA hybrid. *J. Am. Chem. Soc.* 127, 4910-4920 (2005).

50. Noy, A., Perez, A., Lankas, F., Javier Luque, F. and Orozco, M. Relative flexibility of DNA and RNA: a molecular dynamics study. *J. Mol. Biol.* 343, 627-638 (2004).

51. Perez, A., Noy, A., Lankas, F., Luque, F. J. and Orozco, M. The relative flexibility of B-DNA and A-RNA duplexes: database analysis. *Nucleic Acids Res.* 32, 6144-6151 (2004).

52. Orozco, M., Perez, A., Noy, A. and Luque, F. J. Theoretical methods for the simulation of nucleic acids. *Chem Soc Rev* 32, 350 (2003).

Academic References

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