Curriculum Vitae

Alessandro Cembran

Assistant Professor
Department of Chemistry and Biochemistry
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EDUCATION

2004	Ph.D. Computational Chemistry. Department of Chemistry, University of Bologna, Italy.
2000	MS Chemistry, *cum laude*. Department of Chemistry, University of Bologna, Italy

PROFESSIONAL APPOINTMENTS

2015 – date	Graduate Faculty, Integrated Biological Sciences Program, U of MN Duluth
2014 – date	Graduate Faculty, Department of Chemistry and Biochemistry, U of MN Duluth
2014 – date	Assistant Professor, Department of Chemistry and Biochemistry, U of MN Duluth
2009 – 2014	Research Associate, Department of Chemistry, U of MN Twin Cities
2004 – 2009	Postdoctoral Associate, Department of Chemistry, U of MN Twin Cities

PUBLICATIONS

Refereed Journal Articles

1. Lewis, A. K., Dunleavy, K., Senkow, T. L., Her, C., Horn, B. T., Jersett, M. A., Mahling, R., McCarthy, M. R., Perell, G. T., Valley, C. C., Karim, C. B., Gao, J.,

Pomerantz, W. C., Thomas, D. D., Cembran, A. C., Hinderliter, A., and Jonathan N. Sachs. Oxidation increases the strength of the methionine-aromatic interaction. *Nature Chemical Biology*, In Press.

2. Kim, J., Masterson, L. R., Cembran, A., Verardi, R., Shi, L., Gao, J., Taylor, S. S., Veglia, G. (2015) Dysfunctional conformational dynamics of protein kinase A induced by a lethal mutant of phospholamban hinder phosphorylation. *Proceedings of the National Academy of Sciences of the United States of America,* 112, 3716-3721.
3. Srivastava, A. K., McDonald, L. R., Cembran, A., Kim, J., Masterson, L. R., McClendon, C. L., Taylor, S. S., Veglia, G. (2014) Synchronous opening and closing motions are essential for cAMP-dependent protein kinase A signaling. *Structure,* 22, 1-9.
4. Desai, B. J., Goto, Y., Cembran, A., Fedorov, A. A., Almo, S. C., Gao, J., Suga, H., Gerlt, J. A. (2014) Investigating the role of a backbone to substrate hydrogen bond in OMP decarboxylase using a site-specific amide to ester substitution. *Proceedings of the National Academy of Sciences of the United States of America,* 111, 15066-15071.
5. Cembran, A., Kim, J., Gao, J., Veglia, G. (2014) NMR mapping of protein conformational landscapes using coordinated behavior of chemical shifts upon ligand binding. *Physical Chemistry Chemical Physics*, 16, 6508-6518.
6. Veglia, G., Cembran, A. (2013) Role of conformational entropy in the activity and regulation of the catalytic subunit of protein kinase A. *FEBS Journal*, 280, 5608-5615.
7. Yu, T., Higashi, M., Cembran, A., Gao, J., Truhlar, D. (2013) Concerted hydrogen atom and electron transfer mechanism for catalysis by lysine-specific demethylase. *The Journal of Physical Chemistry B, 117*, 8422-8429.
8. Fan, Y., Cembran, A., Ma, S., and Gao, J. (2013) Connecting protein conformational dynamics with catalytic function as illustrated in dihydrofolate reductase. *Biochemistry, 52*, 2036–2049.
9. Cembran, A., Masterson, L. R., McClendon, C. L., Taylor, S. S., Gao, J., and Veglia, G. (2012) Conformational equilibrium of N-myristoylated cAMP-dependent protein kinase A by molecular dynamics simulations. *Biochemistry, 51*, 10186–10196.
10. Cembran, A., Provorse, M. R., Wang, C., Wu, W., and Gao, J. (2012) The third dimension of a More O'Ferrall-Jencks diagram for hydrogen atom transfer in the isoelectronic hydrogen exchange reactions of $(PhX)_2H^{\bullet}$ with X = O, NH, and CH_2. *Journal of Chemical Theory and Computation, 8*, 4347–4358.
11. Masterson, L. R., Cembran, A., Shi, L., and Veglia, G. (2012) Allostery and binding cooperativity of the catalytic subunit of protein kinase A by NMR spectroscopy

and molecular dynamics simulations. *Advances in Protein Chemistry and Structural Biology, 87*, 363–389.

12. Valley, C. C., Cembran, A., Perlmutter, J. D., Lewis, A. K., Labello, N. P., Gao, J., and Sachs, J. N. (2012) The methionine-aromatic motif plays a unique role in stabilizing protein structure. *The Journal of Biological Chemistry, 287*, 34979–34991.
13. Wang, Y., Sosa, C. P., Cembran, A., Truhlar, D. G., and Gao, J. (2012) Multilevel X-Pol: a fragment-based method with mixed quantum mechanical representations of different fragments. *The Journal of Physical Chemistry B, 116*, 6781–6788.
14. Fleisher, A. J., Young, J. W., Pratt, D. W., Cembran, A., and Gao, J. (2011) Flickering dipoles in the gas phase: structures, internal dynamics, and dipole moments of β-naphthol-H_2O in its ground and excited electronic states. *The Journal of Chemical Physics, 134*, 114304.
15. Altoè, P., Cembran, A., Olivucci, M., and Garavelli, M. (2010) Aborted double bicycle-pedal isomerization with hydrogen bond breaking is the primary event of bacteriorhodopsin proton pumping. *Proceedings of the National Academy of Sciences of the United States of America, 107*, 20172–20177.
16. Cembran, A., Bao, P., Wang, Y., Song, L., Truhlar, D. G., and Gao, J. (2010) On the interfragment exchange in the X-Pol method. *Journal of Chemical Theory and Computation, 6*, 2469–2476.
17. Cembran, A., Payaka, A., Lin, Y., Xie, W., Mo, Y., Song, L., and Gao, J. (2010) A non-orthogonal block-localized effective hamiltonian approach for chemical and enzymatic reactions. *Journal of Chemical Theory and Computation, 6*, 2242–2251.
18. Gao, J., Cembran, A., and Mo, Y. (2010) Generalized X-Pol theory and charge delocalization states. *Journal of Chemical Theory and Computation, 6*, 2402–2410.
19. Mazack, M. J. M., Cembran, A., and Gao, J. (2010) Internal dynamics of a coarse-grained protein using analytical harmonic representation. *Journal of Chemical Theory and Computation, 6*, 3601–3612.
20. Becucci, L., Cembran, A., Karim, C. B., Thomas, D. D., Guidelli, R., Gao, J., and Veglia, G. (2009) On the function of pentameric phospholamban: ion channel or storage form? *Biophysical Journal, 96*, L60–L62.
21. Cembran, A., Song, L., Mo, Y., and Gao, J. (2009) Block-localized density functional theory (BLDFT), diabatic coupling, and their use in valence bond theory for representing reactive potential energy surfaces. *Journal of Chemical Theory and Computation, 5*, 2702–2716.
22. Shi, L., Cembran, A., Gao, J., and Veglia, G. (2009) Tilt and azimuthal angles of a transmembrane peptide: a comparison between molecular dynamics calculations and solid-state NMR data of sarcolipin in lipid membranes. *Biophysical Journal, 96*, 3648–3662.

23. Shi, L., Traaseth, N. J., Verardi, R., Cembran, A., Gao, J., and Veglia, G. (2009) A refinement protocol to determine structure, topology, and depth of insertion of membrane proteins using hybrid solution and solid-state NMR restraints. *Journal of Biomolecular NMR, 44*, 195–205.
24. Cembran, A., and Gao, J. (2007) Potential energy functions for an intramolecular proton transfer reaction in the ground and excited state. *Theoretical Chemistry Accounts: Theory, Computation, and Modeling, 118*, 211–218.
25. Cembran, A., González-Luque, R., Serrano-Andrés, L., Merchán, M., and Garavelli, M. (2007) About the intrinsic photochemical properties of the 11-*cis* retinal chromophore: computational clues for a trap state and a lever effect in rhodopsin catalysis. *Theoretical Chemistry Accounts: Theory, Computation, and Modeling, 118*, 173–183.
26. Ha, K. N., Traaseth, N. J., Verardi, R., Zamoon, J., Cembran, A., Karim, C. B., Thomas, D. D., and Veglia, G. (2007) Controlling the inhibition of the sarcoplasmic Ca^{2+}-ATPase by tuning phospholamban structural dynamics. *The Journal of Biological Chemistry 282*, 37205–37214.
27. Cembran, A., and Gao, J. (2006) Excited state intramolecular proton transfer in 1-(trifluoroacetylamino) naphthaquinone: a CASPT2//CASSCF computational study. *Molecular Physics, 104*, 943–955.
28. Cembran, A., Bernardi, F., Olivucci, M., and Garavelli, M. (2005) The retinal chromophore/chloride ion pair: Structure of the photoisomerization path and interplay of charge transfer and covalent states. *Proceedings of the National Academy of Sciences of the United States of America, 102*, 6255–6260.
29. Cembran, A., González-Luque, R., Altoè, P., Merchán, M., Bernardi, F., Olivucci, M., and Garavelli, M. (2005) Structure, spectroscopy, and spectral tuning of the gas-phase retinal chromophore: the β-ionone "handle" and alkyl group effect. *The Journal of Physical Chemistry A, 109*, 6597–6605.
30. Cembran, A., Bernardi, F., Olivucci, M., and Garavelli, M. (2004) Counterion controlled photoisomerization of retinal chromophore models: a computational investigation. *Journal of the American Chemical Society, 126*, 16018–16037.
31. Ferré, N., Cembran, A., Garavelli, M., and Olivucci, M. (2004) Complete-active-space self-consistent-field/Amber parameterization of the Lys296-retinal-Glu113 rhodopsin chromophore-counterion system. *Theoretical Chemistry Accounts: Theory, Computation, and Modeling, 112*, 335–341.
32. Cembran, A., Bernardi, F., Garavelli, M., Gagliardi, L., and Orlandi, G. (2004) On the mechanism of the *cis-trans* isomerization in the lowest electronic states of azobenzene: S_0, S_1, and T_1. *Journal of the American Chemical Society, 126*, 3234–3243.

33. Gagliardi, L., Orlandi, G., Bernardi, F., Cembran, A., and Garavelli, M. (2004) A theoretical study of the lowest electronic states of azobenzene: the role of torsion coordinate in the *cis-trans* photoisomerization. *Theoretical Chemistry Accounts: Theory, Computation, and Modeling, 111*, 363–372.
34. Migani, A., Sinicropi, A., Ferré, N., Cembran, A., Garavelli, M., and Olivucci, M. (2004) Structure of the intersection space associated with Z/E photoisomerization of retinal in rhodopsin proteins. *Faraday Discussions, 127*, 179–91.
35. Cembran, A., Bernardi, F., Olivucci, M., and Garavelli, M. (2003) Excited-state singlet manifold and oscillatory features of a nonatetraeniminium retinal chromophore model. *Journal of the American Chemical Society, 125*, 12509–12519.
36. Ruiz, D. S., Cembran, A., Garavelli, M., Olivucci, M., and Fuss, W. (2002) Structure of the conical intersections driving the *cis-trans* photoisomerization of conjugated molecules. *Photochemistry and Photobiology, 76*, 622–633.
37. Garavelli, M., Bernardi, F., Cembran, A., Castaño, O., Frutos, L. M., Merchán, M., and Olivucci, M. (2002) Cyclooctatetraene computational photo-and thermal chemistry: a reactivity model for conjugated hydrocarbons. *Journal of the American Chemical Society, 124*, 13770–13789.

Book Chapters

1. Gao, J., Wong, K.-Y., Major, D. T., Cembran, A., Song, L., Lin, Y., Fan, Y., and Ma, S. Kinetic isotope effects from hybrid classical and quantum path integral computations. In *Quantum Tunnelling in Enzyme-Catalysed Reactions*, Alleman, R. K., Scrutton, N. S., Eds.; RSC: Cambridge, 2009; pp 105–131.
2. Wong, K.-Y., Song, L., Xie, W., Major, D. T., Lin, Y.-L., Cembran, A., and Gao, J. Quantum Mechanical Methods for Biomolecular Simulations. In *Multi-scale Quantum Models for Biocatalysis*, York, D. M., Lee T.-S., Eds.; Springer: New York, 2009; pp 79–101.
3. Garavelli, M., Bernardi, F., and Cembran, A. Computation of photochemical reaction mechanisms in organic chemistry. In *Computational Photochemistry*, Olivucci M. Ed.; Elsevier: Amsterdam, 2005; pp 191–223.

GRANTS AND AWARDS

2005 – 2006 University of Minnesota Supercomputing Institute Research Scholarship

PROFESSIONAL MEETINGS

Panels Organized

2016 Co-Chair. Platform: Protein-Dynamics and Allostery I. 60th Annual Meeting of the Biophysical Society, Los Angeles, CA.

Conference Presentations

2016 A. Cembran, A. Hinderliter, B. T. Horn, C. T. Pederson, Schneider, K. L., Skogstad, J. A. Hydrophobic interactions elicit cooperative response in dystrophin. 60th Annual Meeting of the Biophysical Society, Los Angeles, CA.

2015 A. Cembran, A. Hinderliter, B. T. Horn, C. T. Pederson, Schneider, K. L., Skogstad, J. A. Hydrophobic interactions elicit cooperative response in dystrophin (poster). 29th Gibbs Conference on Biological Thermodynamics, Carbondale, IL.

2015 Cembran, A., Dicke, A. A., De Simone, A., Mote, K. R., Vostrikov, V., Veglia, G. Sarcolipin-mediated regulation of SERCA by computer simulations (poster). 59th Annual Meeting of the Biophysical Society, Baltimore, MD.

2014 Cembran, A., Vostrikov, V., Veglia, G. Sarcolipin-mediated regulation of SERCA by computer simulations (poster). Chemistry Biology Interface Training Grant Symposium, Minneapolis, MN.

2014 Cembran, A., Veglia, G. Quantitative Interpretation of Chemical Shifts Enables Mapping Proteins Conformational Landscape (poster). 58th Annual Meeting of the Biophysical Society, San Francisco, CA.

2013 Cembran, A., Veglia, G, Gao, J. Computer Simulations of Protein Kinase A (poster). Technical Meeting on High-Throughput Molecular Dynamics, Barcelona, Spain.

2013 Cembran, A., Veglia, G., Gao, J. Computer Simulations of Protein Kinase A (poster). Frontiers in Dynamics Simulations of Biological Molecules, Barcelona, Spain.

2013 Cembran, A., Gao, J., Veglia, G. Computer Simulations of Protein Kinase A. Rise of the Machines: Integration of Experiment, Simulation and Theory for a Mechanistic Understanding of Biomolecular Machines, Telluride, CO.

2013 Cembran, A., Veglia, G. Principal Component Analysis of NMR Chemical Shifts Quantitatively Measures the Equilibrium Shift Induced by Nucleotide Binding to Protein Kinase A (poster). Chemistry Biology Interface Training Grant Symposium, Minneapolis, MN.

2012 Cembran, A., Masterson, L. R., Veglia, G., Gao, J. Computer Simulations of Protein Kinase A Unveil the Structural and Dynamical Effects of N-

Myristoylation (poster). Minnesota Supercomputing Institute Research Exhibition, Minneapolis, MN.

2011 Cembran, A., Gao, J. Block-Localized Wavefunction: A Powerful Tool to Investigate Intermolecular Interactions (poster). 9th Congress of the World Association of Theoretical and Computational Chemists, Santiago de Compostela, Spain.

2010 Cembran, A., Gao, J. Orotidine Monophosphate Decarboxylase Catalysis Dissected (poster). Gordon Research Conferences – Isotopes in Biological & Chemical Sciences, Galveston, TX.

2009 Cembran, A., Gao, J. Orotidine Monophosphate Decarboxylase: a Simple Reaction in a Complex Environment. Molecular Modeling 2009 Meeting, Surfers Paradise, Queensland, Australia.

2008 Cembran, A., Gao, J. Orotidine Monophosphate Decarboxylase: a Simple Reaction in a Complex Environment. XXVIII Midwest Enzyme Chemistry Conference, Chicago, IL.

2008 Cembran, A., Gao, J. QM/MM Study of the Hydride Transfer Reaction Catalyzed by Dihydrofolate Reductase. Mechanistic Analysis of Biological Systems with Novel Computational Models, Telluride, CO.

2002 Cembran, A., Bernardi, F, Garavelli, M. A Computational Study of the Counterion Effect on Retinal Model Photochemistry. 27th Symposium of the Italian Chemical Society National Division of Organic Chemistry, Rome, Italy.

2001 Cembran, A., Bernardi, F, Garavelli, M. A Computational Study of the Counterion Effect on Retinal Model Photochemistry (poster). 1st Sigma Aldrich Young Chemists Symposium, Riccione, Italy

TEACHING EXPERIENCE

Department of Chemistry and Biochemistry, University of Minnesota Duluth

Physical Chemistry II	(Sp 2015, Sp 2016)
Physical Chemistry Laboratory I	(F 2015)
Computational Chemistry	(F 2014)

Department of Chemistry, St. Catherine University

Physical Chemistry I with Lab	(F 2012)

Pedagogical Training Attended

Swenson College of Science and Engineering Flipped Class Cohort, U of MN Duluth (Su 2016)
Swenson College of Science and Engineering Active Learning Cohort, U of MN Duluth (Sp 2016)
Making Comments Count: Providing Feedback on Writing That's Efficient for You and Effective for Students Workshop, U of MN Duluth (F 2015)
Flipped Class Workshop, U of MN Duluth (Sp 2015)
Early Career Workshop Series in Teaching and Learning, U of MN Duluth (F 2104)
Practicum for Future Faculty, U of MN Twin Cities (F 2008)
Teaching in Higher Education, U of MN Twin Cities (Sp 2008)

TEACHING GRANTS

2016 A. Cembran. Flipping the Spin: Active Learning Quantum Mechanics. Swenson College of Science and Engineering Dean's Active Learning Grants Program ($500).
2016 R. Lakhan, A. Cembran, K. Kallevig, B. Tsai. Individual Plan for Student Success. U of MN Duluth Student Success and Retention Small Grant ($2000).

STUNDENT MENTORING

Graduate Students – Current

2014 – date Benjamin T. Horn (co-Adviser)
2015 – date Anthony T. Meger (co-Adviser)
2015 – date Adam M. Jersett

Graduate Committee Member

2015 Andrew K. Lewis (U of MN Twin Cities)

Undergraduate Students – Current

2014 – date Matthew L. Terhaar (1 credit, research volunteer)
2016 – date Alida Besch (SURP $4,500).
2016 – date Bryan J. Reutzel (research volunteer)
2016 – date Nick J. Ruha (research volunteer)

2016 – date Nicole D. Widen (research volunteer)

Undergraduate Students – Graduated

2016 Caitlin T. Pederson (UROP $1,400, research volunteer)
2016 Jesse A. Skogstad (UROP $1,400, research volunteer)
2015 Katie L. Schneider (research volunteer)

Undergraduate Advising

Academic adviser for about 15 chemistry and biochemistry majors every semester.

MANUSCRIPT REVIEW

Theoretical Chemistry Accounts (9), Journal of Chemical Theory and Computation (3), Scientific Reports (1), Journal of the American Chemical Society (1), The Journal of Physical Chemistry (1), The Journal of Physical Chemistry Letters (1), Journal of Physical Organic Chemistry (1), European Biophysics Journal (1), Archives of Biochemistry and Biophysics (1), RSC Advances (1), Bioelectrochemistry (1)

OUTREACH

2016 Northeast Regional Science Fair. Judge.
2014, 2016 Swenson College of Science and Engineering – Science Day. Co-organizer.

CONSULTING

2010 – 2011 Syntiron LLC

PROFESSIONAL MEMBERSHIPS

2014 – date Interdisciplinary Life Sciences Consortium (ILSC) - UMD
2013 – date Biophysical Society
2008 – date American Chemical Society