

LELA VUKOVIĆ

Department of Chemistry and Biochemistry
University of Texas at El Paso
Chemistry & Computer Science Building, Rm 2.0308
500 W. University Ave, El Paso, TX 79968 USA

Phone: (312) 752-8002
E-mail: Lvukovic@utep.edu
Web: <http://utminers.utep.edu/lvukovic>

EMPLOYMENT AND EDUCATION

- 01/2016 –** University of Texas at El Paso
Assistant Professor of Chemistry
- 12/2012 – 12/2015** University of Illinois at Urbana-Champaign
Postdoctoral Fellow, NSF Frontier Center for the Physics of Living Cells
Postdoctoral advisor: Prof. Klaus Schulten
- 08/2007 – 10/2012** University of Illinois at Chicago
Ph.D. Physical Chemistry
- 08/2001 – 05/2005** University of Illinois at Chicago
B. Sc. Chemistry, minor in Mathematics, *summa cum Laude*

OTHER RESEARCH EXPERIENCE

- 09/2011 – 08/2012** Max Planck Institute for Biophysical Chemistry, Göttingen, Germany
Visiting researcher, Theoretical and Computational Biophysics Group
- 05/2005 – 09/2005** Argonne National Laboratory, Argonne, IL
Visiting researcher

FUNDING

- NIH R03 AI142553-01 Vukovic (PI) 11/15/2018 – 10/31/2020
Computational modeling of broad-spectrum non-toxic antiviral nanoparticles with a virucidal inhibition mechanism (role: PI), \$151,000; no-cost extension 10/31/2021

COMPUTER TIME ALLOCATIONS

- 2018 Blue Waters allocation for “Broadening Participation” Vukovic (PI) 03/2018 – 12/2019
Computational modeling of ring-like DNA-nanotube sensors of neurotransmitters (role: PI), 200,000 node hours
- Anton2 supercomputing time, Pittsburgh Supercomputing Center Vukovic (PI) 2016 – 2017
RNA Recognition by the Exosome Complex (role: PI), 200,000 MD simulation units

PUBLICATIONS

Key group publications at UTEP:

11. A. Ekanayake, L. Sobze, **P. Kelich**, J. Youk, N. Bennett, R. Mukherjee, A. Bhardwaj, F. Wuest, **L. Vuković**, R. Derda. Genetically encoded fragment-based discovery (GE-FBD) from phage-displayed macrocyclic libraries with genetically-encoded unnatural pharmacophores, revised and resubmitted to J. Am. Chem. Soc. (2021).
10. **A. Alizadehmojarad**, B. Fazelabdolabadi, **L. Vuković***, Surfactant-controlled mobility of oil droplets in mineral nanopores, *Langmuir*, 36, 12061-12067 (2020).
9. **A. A. Alizadehmojarad**, X. Zhou, A. G. Beyene, **K. E. Chacon**, Y. Sung, R. L. Pinals, M. P. Landry*, **L. Vuković***, Binding affinity and conformational preferences influence kinetic stability of short oligonucleotides on carbon nanotubes, *Advanced Materials Interfaces*, 2000353 (2020).
8. **P. Chaturvedi**, Y. Han, P. Král*, **L. Vuković***, Adaptive evolution of peptide inhibitors for mutating SARS-CoV-2, *Advanced Theory & Simulations*, 3, 2000156 (2020).

7. **P. Chaturvedi**, **L. Vuković***, Structural properties of small single-stranded circular nucleic acids, *J. Phys. Chem. B*, 123, 8216 (2019).
6. **T. A. Nitka**, P. Král, **L. Vuković***, Configurations of nanocubes floating and clustering on liquid surfaces, *J. Phys. Chem. Lett.*, 10, 3592 (2019).
5. R. Nißler, F. A. Mann, **P. Chaturvedi**, J. Horlebein, D. Meyer, **L. Vuković**, S. Kruss, Quantification of the number of adsorbed DNA molecules on single-walled carbon nanotubes, *J. Phys. Chem. C* 123, 4837 (2019).
4. A. G. Beyene+, **A. A. Alizadehmojarad**+, G. Dorlhiac, A. M. Streets, P. Král, **L. Vuković***, M. P. Landry*, Ultralarge modulation of fluorescence by neuromodulators in carbon nanotubes with self-assembled oligonucleotide rings, *Nano Lett.* 18, 6995 (2018). (+ co-first authors)
3. E. Polo, **T. T. Nitka**, E. Neubert, L. Erpenbeck, **L. Vuković**, S. Kruss, Control of integrin affinity by confining RGD peptides on fluorescent carbon nanotubes, *ACS Appl. Mater. Interfaces*, 10, 17693-17703 (2018).
2. **S. Gorle**, Y. Pan, Z. Sun, L. Shlyakhtenko, Y. Lyubchenko*, **L. Vuković***. "Computational Model and Dynamics of Monomeric Full-Length APOBEC3G," *ACS Central Science* 3, 1180-1188 (2017).
1. S. Kruss, D. Salem, **L. Vuković**, B. Lima, E. van der Ende, E. Boyden, M. Strano. "High Resolution Imaging of Cellular Dopamine Efflux Using a Nanosensor Array." *Proc. Natl. Acad. Sci. USA* 114, 1789-1794 (2017).

Other publications while at UTEP:

8. S. T. Jones, V. Cagno, M. Janecek, D. Ortiz, N. Gasilova, D. Constant, Y. Han, **L. Vuković**, P. Král, L. Kaiser, S. Huang, S. Constant, K. Kirkegaard, F. Stellacci, and C. Tapparel, Modified Cyclodextrins as Broad-spectrum Antivirals, *Science Advances*, 6, eaax9318 (2020).
7. L. Zheng, H. Zhao, Y. Han, **L. Vuković**, J. Mecinović, P. Král, and W. T. S. Huck, Catalytic transport of molecular cargo using diffusive binding along a polymer track, *Nature Chemistry* 11, 359 (2019).
6. S. Mondal, G. Jacoby, M. R. Sawaya, Z. A. Arnon, L. Adler-Abramovich, **L. Vuković**, P. Rehak, L. J. W. Shimon, P. Král, R. Beck, D. Eisenberg, and E. Gazit, Transition of metastable cross-alpha crystals into cross-beta fibrils by beta-turn flipping, *J. Am. Chem. Soc.* 141, 363 (2019).
5. S. Shaham-Niv, P. Rehak, D. Zaguri, A. Levin, L. Adler-Abramovich, **L. Vuković**, P. Král, E. Gazit, Differential inhibition of metabolite amyloid formation by generic fibrillation-modifying polyphenols, *Comm. Chem.* 1, 25 (2018).
4. S. Sen, Y. Han, P. Rehak, **L. Vuković***, and P. Král*, Computational Studies of Micellar and Nanoparticle Nanomedicines, *Chem. Soc. Rev.*, 47, 3849-3860 (2018).
3. V. Cagno, P. Andreozzi, M. D'Alicarnasso, P. J. Silva, M. Mueller, M. Galloux, R. Le Goffic, S. T. Jones, M. Vallino, J. Hodek, J. Weber, S. Sen, Dr. E. R. Janecek, A. Bekdemir, B. Sanavio, C. Martinelli, M. Donalisio, M.-A. Rameix-Welti, Y. Han, L. Kaiser, **L. Vuković**, P. Král, C. Tapparel, S. Krol, D. Lembo, F. Stellacci, "Broad-spectrum non-toxic antiviral nanoparticles with a virucidal inhibition mechanism," *Nature Materials*, 17, 195-203 (2018).
2. T. Udayabhaskararao, T. Altantzis, L. Houben, M. Coronado-Puchau, J. Langer, R. Popovitz-Biro, L. M. Liz-Marzán, **L. Vuković**, P. Král, S. Bals, R. Klajn. "Tunable Porous Nanoallotropes Prepared from Binary Nanoparticle Superlattices Self-Assembled at the Solvent-Air Interface," *Science*, 358, 514-518 (2017).
1. S. Shaham-Niv, P. Rehak, **L. Vuković**, L. Adler-Abramovich, P. Král, E. Gazit. "Formation of apoptosis-inducing amyloid fibrils by tryptophan." *Isr. J. Chem.* 57, 729-737 (2017).

Prior to joining UTEP:

19. **L. Vuković***, D. L. Makino, C. Chipot, E. Conti, K. Schulten. "Molecular mechanism of processive 3' to 5' RNA translocation in the active subunit of the RNA exosome complex." *J. Am. Chem. Soc.* 138, 4069-4078 (2016).
18. Y. Zhang*, **L. Vuković***, T. Rudack*, W. Han, K. Schulten. "Recognition of poly-ubiquitins by the proteasome through protein re-folding guided by electrostatic and hydrophobic interactions." *J. Phys. Chem. B* 120, 8137-8146 (2016). (* equal contribution)
17. X. Wang, **L. Vuković**, H. R. Koh, K. Schulten, S. Myong. "Dynamic profiling of double-stranded RNA binding proteins," *Nucl. Acids Res.*, 43, 7566-7576 (2015).
16. M. Landry, **L. Vuković**, S. Kruss, G. Bisker, A. M. Landry, R. Jain, K. Schulten, M. S. Strano. "Comparative Dynamics and Sequence Dependence of DNA and RNA Binding to Single Walled Carbon Nanotubes," *J. Phys. Chem. C*, 119, 10048-10058 (2015).
15. Y. Qiu, H. Niu, **L. Vuković**, P. Sung, S. Myong. "Molecular mechanism of resolving trinucleotide repeat hairpin by helicases," *Structure*, 23, 1018-1027 (2015).
14. **L. Vuković**, H. R. Koh, S. Myong, K. Schulten, "Substrate recognition and specificity of double-stranded RNA binding proteins," *Biochemistry*, 53, 3457-3466 (2014).

13. **L. Vuković**, E. Vokac and P. Král, "Molecular Friction-Induced Electrokinetic Phenomena in Thin Nanotubes," *J. Phys. Chem. Lett.* **5**, 2131-2137 (2014).
12. C. R. James, A. M. Rush, T. Insley, **L. Vuković**, P. Král, and N. C. Gianneschi, "(Poly-oligonucleotide)," *J. Am. Chem. Soc.* **136**, 11216-11219 (2014).
11. **L. Vuković**, A. Madriaga, A. Kuzmis, A. Banerjee, A. Tang, K. Tao, N. Shah, P. Král, H. Onyuksel, "Solubilization of Therapeutic Agents in Micellar Nanomedicines," *Langmuir*, **29**, 15747-15754 (2013).
10. **L. Vuković**, C. F. Burmeister, P. Král, G. Groenhof, "Control Mechanisms of Photo-isomerization in Protonated Schiff Bases," *J. Phys. Chem. Lett.* **4**, 1005-1011 (2013).
9. H. Chan, A. Demortière, **L. Vuković**, P. Král, C. Petit, "Colloidal Nanocube Supercrystals Stabilized by Multipolar Coulombic Coupling," *ACS Nano* **6**, 4203 (2012).
8. J. W. Bae, R. M. Pearson, N. Patra, S. Sunoqrot, **L. Vuković**, P. Král, S. Hong, "Dendron-mediated Self-assembly of Highly PEGylated Block Copolymers: A Potential Nanocarrier Platform," *Chem. Comm.* **47**, 10302 (2011).
7. **L. Vuković**, F. A. Khatib, S. P. Drake, A. Madriaga, K. S. Brandenburg, P. Král, H. Onyuksel, "Highly PEGylated Sterically Stabilized Micelles in Aqueous Media," *J. Am. Chem. Soc.* **133**, 13481-13488 (2011).
6. J. He, X.-M. Lin, H. Chan, **L. Vuković**, P. Král, H. Jaeger, "Diffusion and Filtration Properties of Self-Assembled Gold Nanocrystal Membranes," *Nano Lett.* **11**, 2430-2434 (2011).
5. P. Král, **L. Vuković**, N. Patra, B. Wang, A. Titov, "Control of rotary motion at the nanoscale: Motility, self-assembly, actuation," *J. Nanosci. Lett.* **1**, 128-144 (2011).
4. **L. Vuković**, P. Král, "Coulombically Driven Rolling of Nanorods on Water," *Phys. Rev. Lett.* **103**, 246103 (2009).
3. B. Wang, **L. Vuković**, and P. Král, "Nanoscale Rotary Motors Driven by Electron Tunneling," *Phys. Rev. Lett.* **101**, 186808 (2008).
2. **L. Vukovic**, C. J. Jameson, D. N. Sears, "Intermolecular hyperfine tensor for Xe@O₂. Density and temperature dependence of Xe chemical shifts in oxygen gas," *Mol. Phys.* **104**, 1217 (2006).
1. D. N. Sears, **L. Vukovic**, C. J. Jameson, "Xe nuclear magnetic resonance line shapes in channels decorated with paramagnetic centers," *J. Chem. Phys.* **125**, 114708 (2006).

PATENTS

1. R. E. Gerald, R. J. Klingler, J. W. Rathke, R. Diaz, L. Vukovic. NMR characterization of thin films. US Patent 7456630, issued November 25, 2008.
2. R. E. Gerald, R. J. Klingler, J. W. Rathke, R. Diaz, L. Vukovic. Molecule nanoweaver. US Patent 7501483, issued March 10, 2009.
3. R. E. Gerald, L. Vukovic, J. W. Rathke. Apparatus and method for generating a magnetic field by rotation of a charge holding object. US Patent 7602181, issued October 13, 2009.
4. R. E. Gerald, R. J. Klingler, J. W. Rathke, R. Diaz, L. Vukovic. NMR characterization of thin films. US Patent 7737691B2, issued June 15, 2010.

BOOK CHAPTERS AND CONFERENCE PROCEEDINGS

1. S. Gorle and L. Vuković. "Nanoscale dynamics and energetics of proteins and protein-nucleic acid complexes in classical molecular dynamics simulations." In *Methods in Molecular Biology: Nanoimaging*, Springer Nature, in press, 2018.
2. P. Král, L. Vuković. "Computational Studies of Highly PEG-ylated Sterically Stabilized Micelles: Self-Assembly and Drug Solubilization." In A. Prokop, et al., editors, *Fundamental Biomed. Technol.: Intracellular Delivery*, chapter 16, pp 313-326. Springer, 2014.
3. P. Kral, L. Vuković, N. Patra, B. Wang, A. Titov, "Control of rotary motion at the nanoscale: Motility, self-assembly, actuation." In *Beilstein Bozen Symposium Proceedings of "Functional Nanoscience"*, in Bozen, Italy, May 17-21, 2010.

PRESENTATIONS (*invited)

- "Adaptive Evolution of Peptide Inhibitors for Mutating SARS-CoV-2." Biophysical Society's Virtual Networking Event on Biophysical Approaches to the Development of Therapies for Infectious Disease, October 14, 2020.
- "Multiscale modeling of oligonucleotide-carbon nanotube biosensor platforms." 2019 Southwest and Rocky

Mountain ACS Regional Meeting, El Paso, TX, November 15, 2019.

- “Computational modeling of virucidal inhibition mechanisms of broad-spectrum non-toxic antiviral nanoparticles.” 2019 Southwest and Rocky Mountain ACS Regional Meeting, El Paso, TX, November 15, 2019.
- “Computational modeling of biomedical systems: oligonucleotide-carbon nanotube biosensor platforms and virucidal nanoparticles.” Southwest Theoretical and Computational Chemistry Conference, University of Oklahoma, October 26, 2019. *
- “Self-assembly of functional materials: Exploration with computational experiments.” Faculty for Physical Chemistry, Belgrade, Serbia, May 24, 2019. *
- “From RNA biology to nucleic acid sensors: Exploration with computational experiments.” Contreras group, Department of Chemical Engineering, University of Texas at Austin, May 7, 2019. *
- “Self-assembly of functional materials: Exploration with computational experiments.” Department of Chemistry, Clemson University, September 6, 2018. *
- “Multiscale modeling of DNA-wrapped carbon nanotube nanosensors,” L. Vuković, A. A. Alizadehmojarad. American Chemical Society Meeting, Fall 2018, Boston, MA, August 18-23, 2018.
- “From RNA biology to nucleic acid sensors: Exploration with computational experiments. Department of Chemistry, University of Illinois at Chicago, April 28, 2018. *
- “Modeling of Nanoparticle Superlattices Self-assembly at Liquid-Air Interfaces,” L. Vuković. American Chemical Society Meeting, Spring 2018, New Orleans, LA, March 18-22, 2018.
- “Elucidating mechanisms of RNA- and protein-degradation complexes via molecular dynamics simulations,” L. Vukovic. Department of Chemistry, New Mexico Institute of Mining and Technology, October 27, 2017. *
- “From RNA biology to nucleic acid sensors: Exploration with computational experiments,” L. Vukovic. Department of Biology, University of Texas at El Paso, October 7, 2016. *
- “From RNA biology to nucleic acid sensors: Exploration with computational experiments,” L. Vukovic. Department of Chemistry, University of Goettingen, June 3, 2016. *
- “Computational studies of RNA recognition and translocation in the RNA exosome complex,” L. Vukovic. Department of Structural Cell Biology, Max Planck Institute for Biochemistry, Martinsried, Germany, June 2 24, 2016.
- “From RNA biology to nucleic acid sensors: Exploration with computational experiments,” L. Vukovic. Department of Chemistry, College of Staten Island, City University of New York, February 3, 2015. *
- “From RNA biology to nucleic acid sensors: Exploration with computational experiments,” L. Vukovic. Department of Chemistry, Michigan State University, January 28, 2015. *
- “From RNA biology to nucleic acid sensors: Exploration with computational experiments,” L. Vukovic. Department of Chemistry, Virginia Tech, January 5, 2015. *
- “From RNA biology to nucleic acid sensors: Exploration with computational experiments,” L. Vukovic. Department of Chemistry, University of Texas at El Paso, December 18, 2014. *
- “From self-assembled materials to RNA biology: Exploration and design with computational experiments,” L. Vukovic. Department of Physical Chemistry and Biochemistry, Palacky University, Olomouc, Czech Republic, March 31, 2014. *
- “RNA translocation in the exosome complex investigated by molecular dynamics simulations,” L. Vukovic. Conti lab group meeting, Max Planck Institute for Biochemistry, Martinsried, Germany, March 24, 2014.
- “Substrate recognition and specificity of double-stranded RNA binding proteins,” L. Vukovic, H. R. Koh, S. Myong, K. Schulten. 58th Biophysical Society Meeting, San Francisco, CA, February 15 – 19, 2014.
- “From RNA biology to nanomedicines: Exploration and design with computational experiments,” L. Vukovic. Department of Chemistry and Biochemistry, University of Minnesota - Duluth, MN, February 3, 2014. *
- “From RNA biology to nanomedicines: Exploration and design with computational experiments,” L. Vukovic. Department of Chemistry, Colorado State University, Fort Collins, CO, January 13, 2014. *
- “Nanocarriers based on highly PEG-ylated amphiphiles: Atomistic structure, dynamics, and drug loading,” L. Vukovic. Center for the Physics of Living Cells, University of Illinois at Urbana-Champaign, IL, January 25, 2012. *
- “Highly PEGylated sterically stabilized micelles in aqueous media,” L. Vukovic, S. P. Drake, F. A. Khatib, A. Madriaga, K. S. Brandenburg, P. Kral and H. Onyuksel. American Chemical Society Meeting, Anaheim, CA, March 27 – 31, 2011.
- “Molecular dynamics simulations of SSM nanomedicines: Phase I - computation of static descriptors.” L. Vukovic, A. Madriaga, N. Shah, P. Král and H. Onyuksel. Pacifichem 2010, Honolulu, HI: Dec 15 – 20, 2010.

- "Molecular dynamics simulations of drug solubilization in lipid-based nanomedicines." L. Vukovic, N. Shah, A. Madriaga, P. Král and H. Onyuksel. Leopoldina Symposium: The complexity connecting biomolecular structure and solvation dynamics, Ruhr-Universität Bochum, Bochum, Germany: May 25 – 27, 2010.
- "Mechanical actuators at the nanoscale: molecular propellers, paddles and wheels." L. Vukovic, B. Wang and P. Král. American Physical Society Meeting, Spring 2010, Portland, OR: March 15 –19, 2010.
- "Rotary molecular motion at the nanoscale: motors, propellers, wheels." L. Vukovic, B. Wang and P. Král. American Physical Society March Meeting, Spring 2009, Pittsburgh, PA: March 16 – 20, 2009.
- "Molecular propellers and tunneling-driven motors." L. Vukovic, B. Wang and P. Král. American Physical Society March Meeting, Spring 2008, New Orleans, LA: March 10 – 14, 2008.
- "Intermolecular Hyperfine Tensor for Xe-O₂ and Density and Temperature Dependence of Xe Chemical Shifts in Oxygen Gas." L. Vukovic, C. J. Jameson. ACS Undergraduate Research Symposium, Chicago, IL, February 25, 2005.

POSTER PRESENTATIONS

- L. Vuković, "Computational modeling of novel supramolecular nanomaterials for viral degradation" Gordon Research Conference on Self-Assembly & Supramolecular Chemistry, Les Diablerets, Switzerland, May 19-26 2017.
- L. Vuković. "Elucidating mechanisms of RNA recognition and processing in the exosome complex via enhanced sampling molecular dynamics simulations." American Chemical Society Meeting, Spring 2017, San Francisco, CA, April 1-6, 2017.
- L. Vukovic. "Engineering and optimizing nanosensors for neurotransmitters through computational approaches." Gordon Research Conference on Bioinspired materials, Les Diablerets, Switzerland, June 5-10 2016.
- L. Vukovic, Y. Zhang, T. Rudack, W. Han, K. Schulten. "Recognition of Poly-ubiquitins by the Proteasome through Protein Re-folding Guided by Electrostatic and Hydrophobic Interactions." 60th Biophysical Society Meeting, Los Angeles, CA, February 27-March 2 2016.
- L. Vukovic, D. L. Makino, C. Chipot, E. Conti, K. Schulten. "Molecular mechanism of processive 3' to 5' RNA translocation in the exosome complex." Gordon Research Conference on Nucleic Acids, Biddeford, ME, May 31-June 5, 2015.
- L. Vukovic, D. L. Makino, C. Chipot, E. Conti, K. Schulten. "Molecular mechanism of processive 3' to 5' RNA translocation in the exosome complex." 59th Biophysical Society Meeting, Baltimore, MD, February 7-11 2015.
- T. Rudack, Y. Zhang, L. Vukovic, W. Han, K. Schulten. "Computational Study of Ubiquitin Recruitment and Transport of the 26S Proteasome." 59th Biophysical Society Meeting, Baltimore, MD, February 7-11 2015.
- L. Vukovic, D. L. Makino, C. Chipot, E. Conti, K. Schulten. "Molecular mechanism of processive 3' to 5' RNA translocation in the exosome complex." NSF-Center for the Physics of Living Cells Summer School, Urbana, IL, July 28-29, 2014.
- L. Vukovic, H. R. Koh, S. Myong, K. Schulten, "Substrate recognition and specificity of double-stranded RNA binding proteins," Gordon Research Conference on Nucleic Acids, Biddeford, ME, June 2-7, 2013.
- L. Vukovic, H. R. Koh, S. Myong, K. Schulten, "Substrate recognition and specificity of double-stranded RNA binding proteins," National Science Foundation (NSF) site visit at the Center for the Physics of Living Cells, Urbana, IL, April 25, 2013.
- L. Vukovic, C. Burmeister, P. Král, G. Groenhof, "Photoisomerization control mechanisms in protonated Schiff bases," 57th Biophysical Society Meeting, Philadelphia, PA, February 2-6, 2013.
- L. Vukovic, C. Burmeister, P. Král, G. Groenhof, "Photoinduced isomerization of a small protonated Schiff base: Bond selectivity and quantum yield," American Chemical Society Meeting, Philadelphia, PA, August 17-21, 2012.
- L. Vukovic, C. Burmeister, P. Král, G. Groenhof, "Photoinduced isomerization of a small protonated Schiff base: Bond selectivity and quantum yield," Faraday Discussion 157: Molecular Reaction Dynamics in Gases, Liquids and Interfaces, Assisi, Italy, June 25-27, 2012.
- L. Vukovic, C. Burmeister, P. Král, G. Groenhof, "Photoinduced isomerization of a small protonated Schiff base: Bond selectivity and quantum yield," Hünfeld 2012: Workshop on Computer Simulation and Theory of Macromolecules, Hünfeld, Germany, April 20-21, 2012.
- L. Vukovic, F. A. Khatib, S. P. Drake, A. Madriaga, K. S. Brandenburg, A. T. Tang, N. Shah, P. Král and H. Onyuksel, "Highly PEG-ylated Sterically Stabilized Micelles in Aqueous Media: Structure, Dynamics, and Storage of Therapeutic Agents," Biophysical Society 56th Annual Meeting, San Diego, CA, February 25 – 29, 2012.
- L. Vukovic, S. P. Drake, F. A. Khatib, A. Madriaga, K. S. Brandenburg, P. Kral and H. Onyuksel, "Structure and

Dynamics of Highly PEG-ylated Sterically Stabilized Micelles in Aqueous Media," GDCh Wissenschaftsforum Chemie 2011, Bremen, Germany, September 4-7, 2011.

N. Patra, L. Vukovic, E. Vokac, I. Yzeiri, P. Král, "Transport of ionic solutions through regular and porous nanotubes," American Chemical Society Meeting, Anaheim, CA, March 27 – 31, 2011.

H. Chan, L. Vuković, P. Král, Jinbo He and H. Jaeger, "Modeling Material Properties of Freestanding Nanoparticle Membranes and Capsules," Workshop on Self-Assembled Bio-Inspired Materials for Energy, Argonne National Laboratory, Argonne, IL, February 4 – 5, 2011.

L. Vukovic, N. Shah, A. Madriaga, P. Král and H. Onyuksel. "Molecular dynamics simulations of drug solubilization in lipid-based nanomedicines." From Computational Biophysics to Systems Biology Workshop (CBSB), Traverse City, MI, June 6-8, 2010.

L. Vukovic, N. Shah, A. Madriaga, P. Král and H. Onyuksel. "Molecular dynamics simulations of lipid-based nanomedicines: Drug solubilization in PEGylated phospholipid nanocarriers." 239th American Chemical Society Meeting, San Francisco, CA, March 21-25, 2010.

L. Vukovic, B. Wang and P. Král. "Rotary molecular motion at the nanoscale: motors and propellers." 41st Midwest Theoretical Chemistry Conference, Carbondale, IL, June 2009.

L. Vukovic, B. Wang and Petr Král. "Current-driven Nanofluidic Propellers with Chemically Tunable Blades." Materials Research Society Fall Meeting, Boston, MA, November 26-30, 2007.

R. E. Gerald II, L. Vukovic, R. Diaz, R. J. Klinger and J. W. Rathke. "Molecule Nanoweaver." Rocky Mountain Conference on Analytical Chemistry, Summer 2005, Denver, CO, August 1–4, 2005.

STUDENT AND GROUP MEMBER PRESENTATIONS

- P. Chaturvedi, L. Vukovic, "Structural and dynamical properties of small single stranded circular nucleic acids," 2019 Southwest and Rocky Mountain ACS Regional Meeting, El Paso, TX, November 15, 2019. (talk)
- T. A. Nitka, L. Vukovic, "Modeling of Nanocube Immersion and Self-Assembly at Liquid-Air Interfaces," 2019 Southwest and Rocky Mountain ACS Regional Meeting, El Paso, TX, November 15, 2019. (talk)
- P. Chaturvedi, L. Vukovic, "Structural and dynamical properties of small single stranded circular nucleic acids," Southwest Theoretical and Computational Chemistry Conference, University of Oklahoma, October 26, 2019. (poster)
- T. A. Nitka, L. Vukovic, "Modeling of Nanocube Immersion and Self-Assembly at Liquid-Air Interfaces," Chemistry Research Days, University of Texas at El Paso, El Paso, TX, April 13, 2018. (talk)
- P. Chaturvedi, L. Vukovic, "Structural and dynamical properties of small single stranded circular nucleic acids," Chemistry Research Days, University of Texas at El Paso, El Paso, TX, August 4, 2018. (poster)
- T. T. Nitka, L. Vukovic, "Modeling of Nanoparticle Immersion and Self-assembly at Liquid-Air Interfaces," American Chemical Society Meeting, Fall 2018, Boston, MA, August 18-23, 2018. (poster)
- C. Cuellar, L. Vukovic. "Atomistic modeling of nucleic acid recognition by nucleic acid binding proteins." COURI Summer Symposium, University of Texas at El Paso, El Paso, TX, August 4, 2018. (poster)
- A. A. Alizadehmojarad, L. Vukovic, "Computational modeling of ring DNA-carbon nanotube sensors," Chemistry Research Days, University of Texas at El Paso, El Paso, TX, April 14, 2018. (talk)
- A. Alizadeh-Mojarad, A. G. Beyene, E. Tindall, M. P. Landry, L. Vuković, "Interpreting sensing mechanisms in nucleic acid-wrapped nanotube sensors through computational approaches." American Chemical Society Meeting, Spring 2017, San Francisco, CA, April 1-6, 2017. (talk)
- A. Alizadeh-Mojarad, L. Vuković. "Effects of confinement and composition on oil/water interface in nanopore environment." American Chemical Society Meeting, Spring 2017, San Francisco, CA, April 1-6, 2017. (talk)
- S. Gorle, L. Vukovic. "Model and Dynamics of a Full A3G Monomer." NIH meeting for A3G Structural Biology Related to HIV/AIDS, Bethesda, MD, June 23, 2017. (poster)
- S. Gorle, L. Vukovic. "Resolving structural dynamics and DNA-binding of APOBEC3G protein." 61st Biophysical Society Meeting, New Orleans, LA, February 11-15, 2017. (poster)

WORKSHOPS AND OTHER CONFERENCES

2016 NSF Chemistry Early Career Investigator Workshop, National Science Foundation, Arlington, VA: March 10-11, 2016.

Computational Biophysics Workshop (NAMD / VMD), National Resource for Automated Molecular Microscopy, The

Scripps Research Institute, San Diego, California: July 12-16, 2010.

Dynamics of molecular mechanisms of biological photoreceptors: interplay between experiment and theory, Schloss Ringberg, Tegernsee, Germany: October 9-11, 2011. (not contributed)

MENTORING EXPERIENCE

Postdoctoral researcher:

Suresh Gorle (2016-2018), went on to the postdoctoral position at The University of Texas Medical Branch

Graduate students:

Ali A. Alizadehmojarad (Master degree graduate at UTEP, 2016-2018), currently a PhD student at Rice University

Parth Chaturvedi (PhD student, 2016-2021), to graduate with a PhD in 05/2021

Tara Nitka (PhD student, 2017-2021), to graduate with a PhD in 08/2021

Payam Kelich (PhD student, 2020-)

Huanhuan Zhao (Master student in Bioinformatics program, 2020-)

Undergraduate students:

Carlos Cuellar (2018), currently a PhD student at University of Illinois

Sara Linn (08/2019-12/2019)

Jenny Crager (2020)

Joshua A Silva (09/2020-)

Kevin Chacon (08/2019-)

Student and PI Awards at UTEP:

Ali A. Alizadehmojarad – UTEP College of Science Best Thesis Award, Fall 2018

Prof. Lela Vukovic – UTEP College of Science Faculty Mentoring Award, Fall 2018

Sara Linn - award for academic and research excellence in Chemistry, Fall 2019

SERVICE / OUTREACH

- Reviewer for the *Nature Communications*, *ACS Nano*, *Journal of Chemical Theory & Computation*, *Journal of Physical Chemistry*, *Nucleic Acids Research*, *Scientific Reports*, *Nano Letters*, *J. Am. Chem. Soc.*, *Biophysical Journal*, *J. Mex. Chem. Soc.*, *Bioconjugate Chem.*, *Cell Biochemistry and Biophysics*
- Reviewer for EPSCOR proposals (2018-2021), NSF panel reviewer (2019), NIH NIAID panel reviewer (2020), Swiss National Supercomputing Center (2018, 2019)
- Co-organizing a Chemistry Research Day (Department of Chemistry and Biochemistry, UTEP, 04/2018, 04/2019)
- Served as a committee member for Jeffrey Richards, Aruna Nair, Bianka Holguin, Priyanka Gade, Zhaobo Li, Asiel Mena, and Sharmin Akter (Physics)
- Served as a member of a Chemistry Chair search committee (Department of Chemistry, UTEP, 2019)
- Serving as a member of a library committee (Department of Chemistry, UTEP, 2021 -)
- Serving as a member of a new graduate student committee (Department of Chemistry, UTEP, 2016 -)
- Serving as a member of a UTEP chemistry student awards committee (Department of Chemistry, UTEP, 2016 -)
- Serving as a Chair of a UTEP chemistry graduate student awards committee (Department of Chemistry, UTEP, 2018 - 2019)
- Served as a member of a new faculty search committee (Department of Chemistry, UTEP, 2017-2018; 2020-2021)
- Served as a reviewer at an ASCR Leadership Computing Challenge (ALCC) panel (US DOE, 04/2016)
- Served as a member of the search committee for an Assistant Director of Technology Development and Training (UIUC, 06/2015)
- Organizer of four week-long Computational Biophysics 'Hands On' Workshops in the NIH Center for Macromolecular Modeling and Bioinformatics (02/2015 – 12/2015)
- Performed massive parametrization of molecules for iPad application *Molecules*, an interactive molecular dynamics app for general public based on NAMD and VMD, developed by Theodore Gray (2014).
- Organizer for the Center for the Physics of Living Cells Post-Doc and Graduate Student Symposium (Spring,

2013)

PROFESSIONAL MEMBERSHIP

American Chemical Society, Biophysical Society, Royal Society of Chemistry (RSC) Associate Member