

Ken D. Shimizu (updated 2/2022)

Professor
Department of Chemistry and Biochemistry
University of South Carolina
Columbia, SC 29208

Research Interests: Supramolecular Chemistry, Molecular Recognition, Physical Organic Chemistry, Molecularly Imprinted Polymers, Materials Chemistry

Professional Experience

Appointments

<u>Dates</u>	<u>Title</u>	<u>Institution</u>	<u>Department</u>
1997-2003	Assistant Professor	University of South Carolina	Chemistry
2003-2010	Associate Professor	University of South Carolina	Chemistry
2010-present	Professor	University of South Carolina	Chemistry
2015-2021	Department Chair	University of South Carolina	Chemistry

Education

<u>Institution</u>	<u>Major / Area</u>	<u>Degree & Year</u>
Cornell University	Chemistry	B.A.: 1990
Massachusetts Institute of Technology	Chemistry	Ph.D.: 1995
Boston College	Chemistry	NIH Postdoc Fellow: 1995-1997

Honors and Awards:

SC ACS Chemist of the Year	2015
SERMACS Symposium Organizer: "Supramolecular Chemistry"	2013
Session Chair for Mesilla Workshop on Aromatic Interactions	2011
Editorial Advisory Board: Molecular Imprinting	2011 – present
Co-organizer of 6 th International Molecular Imprinting Conference	2010
Editorial Board Organic Chemistry International	2008 – 2015
Editorial Advisory Board: Journal of Molecular Recognition	2008 – 2012
Mungo Undergraduate Teaching Award	2008
Organized SERMACS session on Functional polymers and biomacromolecules	2006
Japan Society for the Promotion of Science (JSPS) Fellowship	2004
Mortar Board Excellence in Teaching Award	2001
Research Corporation Research Innovation Award	1997
NIH Postdoctoral Fellowship	1995 – 1997
CRC Award for Achievement in Organic Chemistry	1987

4. Research Highlights

Paper on "Hydrogen bond TS stabilization" highlighted in Chemistry World	2020
Cover and Hot article in <i>Organic & Biomolecular Chemistry</i> vol 15	2017
Paper on "Silver-pi interaction" highlighted in <i>ChemistryViews</i> magazine	2015
Paper on "Silver-pi interaction" highlighted in <i>ACS Noteworthy Chemistry</i>	2015
Paper on "Proton Grease" highlighted in <i>RSC Chemistry World</i>	2012
Article on cover of <i>Current Opinion in Chemical Biology</i> vol 14	2010
Interviewed and quoted in <i>Technology Review</i> magazine (June)	2010
Paper (<i>Org. Lett.</i> , 2009 , 11, 2599) highlighted in <i>ACS Noteworthy</i> column Aug	2009
Paper (<i>J. Am. Chem. Soc.</i> , 2009 , 131, 12062) highlighted in <i>Chem. & Eng. News</i> , 87(35)	2009
Paper (<i>Org. Lett.</i> , 2008 , 10, 3547) highlighted in <i>Nature Chem. Aug. 1</i>	2008
Interviewed and quoted in <i>Technology Review</i> magazine (Oct.)	2008
Paper (<i>Chem. Comm</i> , 2007 , 3, 228) highlighted in <i>MRS Bulletin</i> , 32, 302	2007
Paper (<i>Chem. Comm.</i> 2004 , 10, 1172) among 10 most downloaded articles	2004
Paper (<i>Chem. Comm.</i> 2004 , 10, 1172) highlighted in <i>ACS Heartcut</i> , June	2004
ACS meeting presentation highlighted in <i>Chem. & Eng. News</i> , 80(23), 51	2002
Presentation highlighted in <i>MRS Bulletin</i> , 27, 563	2002
Cover article of <i>Analyst</i> vol 125	2000

5. Synergistic Activities

- Research Advisor for 21 Ph.D. graduate students
- Research Advisor for 7 M.S. graduate students
- Research Advisor for 9 high school students in research activities
- Research Advisor for 36 undergraduate students
- NSF LEAP review panel (2022)
- NSF MSN review panel (2020)
- NSF CCI review panel (2016)
- NSF CBET review panel (2015)
- Deutsche Forschungsgemeinschaft (DFG) review panel (2014)
- NSF MSN review panel (2014)
- NSF MSN review panel (2011)
- NSF CBET review panel (2011)
- NSF CBET review panel (2008)
- NSF CBET review panel (2007)
- NSF SBIR review panel (2007)
- NIH SBICA study section 2006
- NIH BCMBIRG study section (2006)
- Faculty mentor for High School lab experience ScienceLab (2008 – present)
- Mentor / research director for 5 Undergraduates in NSF Research Experiences for Undergraduates (REU) Program in Nanoscience.
- Mentor / thesis advisor for the University of South Carolina Honors College.
- Faculty advisor for local South Carolina American Chemical Society Chapter (SACS)

6. Research funding (PI awards)

- NSF, “Molecular rotors for studying transition state stabilization by non-covalent interactions” PI, **\$447,500**, 08/01/2020 - 07/31/2023
- NSF MRI Q-Exactive MS co-PI **\$450,000**, 09/2018 – 08/2019
- EPSCoR, “Collaborative Research Program (CRP): Programmable Polymers Based on Restricted Rotation Formed by Free Radical Polymerization” **\$60,000**, 05/2018 to 04/2019
- NSF, “Comprehensive Models of Non-Covalent Aromatic Interactions” **\$460,000**, 8/2017 to 07/2020
- NSF, “Molecular balance for measuring molecular-level anion effects on amino acids” **\$390,000**, 9/2013 to 09/2016
- EPSCoR, “Collaborative Research Program (CRP): Colorimetric molecular sensors for monitoring stress and strain in synthetic blood vessels” **\$100,000**, 01/2013 to 06/2014
- NSF, “Programmable polymers based on restricted rotation” **\$390,000**, 10/01/2011 to 09/30/2014
- NSF, “US Egypt Cooperative Research: Luminescent Molecularly Imprinted Polymer Sensor Arrays” PI, **\$125,000**, 8/01/2011 to 7/31/2014
- NSF, “A molecular balance for studying the non-covalent interactions of aromatic surfaces” PI, **\$460,000**, 8/01/2009 to 7/31/2013.
- NSF, “New Strategies for Improved Molecularly Imprinted Polymers”, **\$250,000**, 8/15/08 to 8/14/11
- NIH, “New Strategies for Improved Imprinted Polymers”, **\$1,128,906**, 3/01-3/07
- PRF, “New Model Systems to Measure Weak Non-covalent Interactions”, **\$90,000**, 09/01/07 to 08/3/09
- NSF, “Conformationally Programmable Molecular Receptors”, **\$420,000**, 08/06 to 06/09
- NSF, “Conformationally Programmable Molecular Receptors”, **\$399,000**, 07/15/03 to 07/14/06
- NSF, “Synthetic Self-Assembling Polyimides”, **\$370,002**, 9/01/98 – 8/31/03.

7. Publications (99 total; H-index: 45 Google Scholar, 39 Web of Science)

I. Karki, P. Li, E.C. Vik, A. Manzewitsch, E. Divirgilio, W.E. Brewer, K.D. Shimizu, “Absorption properties of monolithic poly (divinylbenzene-co-N-vinylpyrrolidone) over a wide range of monomer ratios”, *Reactive and Functional Polymers*. **2021**, 163, 104888.

P. Li, E. C. Vik, K. D. Shimizu, “N -Arylimide Molecular Balances: A Comprehensive Platform for Studying Aromatic Interactions in Solution.” *Acc. Chem. Res.* **2020**, 53, 2705–2714.

E.C. Vik, P. Li, J.M. Maier, D.O. Madukwe, V.A. Rassolov, P.J. Pellechia, E. Masson, K.D. Shimizu, “Large transition state stabilization from a weak hydrogen bond”, *Chem. Sci.* **2020**, 11, 7487–7494.

E.C. Vik, P. Li, P.J. Pellechia, K.D. Shimizu, “Transition-State Stabilization by $n \rightarrow \pi^*$ Interactions Measured Using Molecular Rotors”, *J. Am. Chem. Soc.* **2019**, 141, 16579–16583

P. Li, E. C. Vik, J. M. Maier, I. Karki, S. M. S. Strickland, J. M. Umana, M. D. Smith, P. J. Pellechia and K. D. Shimizu, “”, *J. Am. Chem. Soc.*, **2019**, 141, 12513–12517.

- J. Hwang, P. Li, E. C. Vik, I. Karki, K. D. Shimizu, "Study of Through-Space Substituent- π interactions using N-Phenylimide Molecular Balances." *Org. Chem. Front.* **2019**, 6, 1266-1271.
- J. M. Maier, P. Li, J. S. Ritchey, C. J. Yehl, K. D. Shimizu, "Anion-enhanced solvophobic effects in organic solvent." *Chem. Commun.* **2018**, 54, 8502–8505.
- J. Hwang, P. Li, M. D. Smith, C. E. Warden, D. A. Sirianni, E. C. Vik, J. M. Maier, C. J. Yehl, C. D. Sherrill, K. D. Shimizu, "Tipping the Balance between S- π and O- π Interactions". *J. Am. Chem. Soc.* **2018**, 140 (41), 13301-13307.
- L. Ping, W. J. Richardson, D. Song and K. D. Shimizu, "Chapter 14: Molecularly Imprinted Polymer Sensor Arrays" in *Molecularly Imprinted Polymers for Analytical Chemistry Applications*; ed. W. Kutner, Royal Society of Chemistry, Cambridge, **2018**.
- J. M. Maier, P. Li, E. C. Vik, C. J. Yehl, S. M. S. Strickland and K. D. Shimizu, "Measurement of Solvent OH- π Interactions Using a Molecular Balance", *J. Am. Chem. Soc.*, **2017**, 139, 6550–6553.
- P. Li, J. M. Maier, E. C. Vik, C. J. Yehl, B. E. Dial, A. E. Rickher, M. D. Smith, P. J. Pellechia and K. D. Shimizu, "Stabilizing Fluorine- π Interactions", *Angew. Chem., Int. Ed.*, **2017**, 56, 7209–7212.
- G. Rushton, E. C. Vik, W. G. Burns, R. D. Rasberry and K. D. Shimizu, "Guest control of a hydrogen bond-catalysed molecular rotor", *Chem. Commun.*, **2017**, 53, 12469–12472.
- J. Hwang, P. Li, K. D. Shimizu. "Synergy between experimental and computational studies of aromatic stacking interactions." *Org. Biomol. Chem.* **2017**, 15, 1554–1564. **(Cover Article and 2017 Hot Article in Organic and Biomolecular Chemistry)**
- K. D. Shimizu, P. Li, J. Hwang. "CHAPTER 5. Solution-Phase Measurements of Aromatic Interactions." in *Monographs in Supramolecular Chemistry* (eds. Johnson, D. W. & Hof, F.) (Royal Society of Chemistry) **2016**, 124–171.
- P. Li; J. M. Maier; J. Hwang; M. D. Smith; J. A. Krause; B. T. Mullis; S. M. S. Strickland; K. D. Shimizu. "Solvent-induced reversible solid-state colour change of an intramolecular charge-transfer complex" *Chem. Commun.*, **2015**, 51, 14809-14812.
- J. M. Maier; P. Li; J. Hwang; M. D. Smith; K. D. Shimizu. "Measurement of Silver- π Interactions in Solution Using Molecular Torsion Balances" *J. Am. Chem. Soc.*, **2015**, 137, 8014-8017.
- J. Hwang; B. E. Dial; P. Li; M. E. Kozik; M. D. Smith; K. Shimizu. "How important are dispersion interactions to the strength of aromatic stacking interactions in solution?" *Chemical Science*, **2015**, 6, 4358-4364.
- P. Li; J. Hwang; J. M. Maier; C. Zhao; D. V. Kaborda; M. D. Smith; P. J. Pellechia; K. D. Shimizu. "Correlation between Solid-State and Solution Conformational Ratios in a Series of N-(o-Tolyl)Succinimide Molecular Rotors." *Cryst. Growth Des. Crystal Growth & Design*, **2015**, 15, 3561-3564.
- P. Li, T. M. Parker, J. Hwang, F. Deng, M. D. Smith, P. J. Pellechia, C. D. Sherrill, K. D. Shimizu. "The CH- π Interactions of Methyl Ethers as a Model for Carbohydrate-N-Heteroarene Interactions." *Org. Lett.*, **2014**, 5064-5067.
- M. J. Maher, K. Yehl, F. Haque, A. Faint, K. D. Shimizu, C. J. Stephenson. "Surprising variations in the rate of ring opening for a series of rhodamine lactams with similar equilibrium endpoints." *Sens. Actuators, B Sensors and Actuators, B: Chemical*, **2014**, 200, 1-8.
- C. Zhao, P. Li, M. D. Smith, P. J. Pellechia, K. D. Shimizu. "Experimental Study of the Cooperativity of CH- π Interactions." *Org. Lett.*, **2014**, 16, 3520-3523.

D. Song, Y. Zhang, M. F. Geer, K. D. Shimizu. "Characterization of molecularly imprinted polymers using a new polar solvent titration method." *J. Mol. Recognit.*, **2014**, 27, 448-457.

J. Hwang, P. Li, W. R. Carroll, P. J. Pellechia, K. D. Shimizu. "Additivity of substituent effects in aromatic stacking interactions." *J. Am. Chem. Soc.*, **2014**, 136, 14060–14067

K. D. Shimizu. "Intermolecular forces: A solution to dispersion interactions." *Nat Chem*, **2013**, 5, 989-990. **(Invited commentary)**

P. Li, C. Zhao, M. D. Smith, K. D. Shimizu. "Comprehensive Experimental Study of N-Heterocyclic pi-Stacking Interactions of Neutral and Cationic Pyridines." *J. Org. Chem.*, **2013**, 78, 5303-5313.

B. E. Dial, P. J. Pellechia, M. D. Smith, K. D. Shimizu. "Proton Grease: An Acid Accelerated Molecular Rotor" *J. Am. Chem. Soc.*, **2012**, 134, 3675-3678.

R. D. Rasberry, K. D. Shimizu. "Molecular Machines" in eds. J. L. Atwood, J. W. Steed, Taylor & Francis, **2012**, *Encyclopedia of Supramolecular Chemistry*

C. Zhao, R. M. Parrish, M. D. Smith, P. J. Pellechia, C. D. Sherrill, K. D. Shimizu. "Do Deuteriums Form Stronger CH-pi Interactions?" *J. Am. Chem. Soc.*, **2012**, 134, 14306-14309.

L. X. Ren, J. Y. Zhang, X. L. Bai, C. G. Hardy, K. D. Shimizu, C. B. Tang. "Preparation of cationic cobaltocenium polymers and block copolymers by "living" ring-opening metathesis polymerization" *Chem Sci*, **2012**, 3, 580-583.

Y. S. Chong, B. E. Dial, W. G. Burns, K. D. Shimizu. "Covalent locking and unlocking of an atropisomeric molecular switch" *Chem. Commun.*, **2012**, 48, 1296-1298.

Y. Zhang, K. D. Shimizu. "Molecular imprinting and sensor development" in *Chemosensors: Principles, Strategies, and Applications*, eds. B. Wang, E. V. Anslyn, John Wiley & Sons, Hoboken, New Jersey, **2011**, pp. 107-120.

W. R. Carroll, C. Zhao, M. D. Smith, P. J. Pellechia, K. D. Shimizu. "A Molecular Balance for Measuring Aliphatic CH-pi Interactions." *Org. Lett.*, **2011**, 13, 4320-4323.

B. E. Dial, R. D. Rasberry, B. N. Bullock, M. D. Smith, P. J. Pellechia, S. Profeta, K. D. Shimizu. "Guest-Accelerated Molecular Rotor." *Org. Lett.*, **2011**, 13, 244-247.

Y. G. Zhang, D. Song, J. C. Brown, K. D. Shimizu. "Suppression of background sites in molecularly imprinted polymers via urea-urea monomer aggregation" *Org. Biomol. Chem.*, **2011**, 9, 120-126.

R. D. Rasberry, K. D. Shimizu. "Molecular Machines" in eds. Taylor & Francis, **2010**, *Encyclopedia of Supramolecular Chemistry*,

K. D. Shimizu, C. J. Stephenson. "Molecularly imprinted polymer sensor arrays" *Curr. Opin. Chem. Biol.*, **2010**, 14, 743-750. **(Cover Article)**

Y. Zhang, D. Song, L. M. Lanni, K. D. Shimizu. "Importance of Functional Monomer Dimerization in the Molecular Imprinting Process." *Macromolecules*, **2010**, 43, 6284-6294.

K. D. Shimizu. "Reading polymer codes." *Nat. Chem.*, **2010**, 2, 612-613. **(Invited commentary)**

C. J. Stephenson, K. D. Shimizu. "A fluorescent diastereoselective molecular sensor for 1,2-aminoalcohols based on the rhodamine B lactone-zwitterion equilibrium" *Org. Biomol. Chem.*, **2010**, 8, 1027-1032.

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- Y. S. Chong, W. R. Carroll, W. G. Burns, M. D. Smith, K. D. Shimizu. "A High-Barrier Molecular Balance for Studying Face-to-Face Arene-Arene Interactions in the Solid State and in Solution" *Chem. Eur. J.*, **2009**, 15, 9117-9126.
- R. D. Rasberry, K. D. Shimizu. "Molecular playdough: conformationally programmable molecular receptors based on restricted rotation" *Org. Biomol. Chem.*, **2009**, 7, 3899-3905.
- Y. Zhang, J. M. Lavin, K. D. Shimizu. "Solvent Programmable Polymers Based on Restricted Rotation" *J. Am. Chem. Soc.*, **2009**, 131, 12062-12063. (**Highlighted in Chem. & Eng. News, 2009, 87(35), 25-26.**)
- R. D. Rasberry, X. Wu, B. N. Bullock, M. D. Smith, K. D. Shimizu. "A small molecule diacid with long-term chiral memory." *Org. Lett.*, **2009**, 11, 2599-2602. (**Highlighted in ACS noteworthy column Aug 31, 2009**)
- X. Wu, K. D. Shimizu. "Development of molecularly imprinted polymers as tailored templates for the solid-state [2+2] photodimerization" *Biosensors and Bioelectronics*, **2009**, 25, 640-646.
- X. G. Wu, K. Goswami, K. D. Shimizu. "Comparison of monofunctional and multifunctional monomers in phosphate binding molecularly imprinted polymers" *J. Mol. Recognit.*, **2008**, 21, 410-418.
- X. Wu, K. D. Shimizu. "Chapter 15. Molecular imprinting for sensor applications." in eds. V. M. Rotello, S. Thayumanavan, John Wiley & Sons, Hoboken, NJ, **2008**, *Molecular Recognition and Polymers*, pp. 395-429.
- W. R. Carroll, P. Pellechia, K. D. Shimizu. "A Rigid Molecular Balance for Measuring Face-to-Face Arene-Arene Interactions" *Org. Lett.*, **2008**, 10, 3547-3550. (**Highlighted in Nature Chem. 2008, Aug**)
- X. Y. Wu, W. R. Carroll, K. D. Shimizu. "Stochastic lattice model Simulations of molecularly imprinted polymers" *Chem. Mater.*, **2008**, 20, 4335-4346.
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- G. T. Rushton, W. G. Burns, J. M. Lavin, Y. S. Chong, P. Pellechia, K. D. Shimizu. "Determination of the rotational barrier for kinetically stable conformational isomers via NMR and 2D TLC - An introductory organic chemistry experiment" *J. Chem. Educ.*, **2007**, 84, 1499-1501.
- C. J. Stephenson, K. D. Shimizu. "Colorimetric and fluorometric molecularly imprinted polymer sensors and binding assays" *Polym. Int.*, **2007**, 56, 482-488.
- J. M. Lavin, K. D. Shimizu. "A supramolecular switch with molecular memory" *Chem. Commun.*, **2007**, 228-230. (**highlighted in MRS Bulletin, 2007, 32, 302**)
- J. M. Lavin, K. D. Shimizu. "Rapid screening of a receptor with molecular memory." *Org. Lett.*, **2006**, 2389-2392.
- K. D. Shimizu. "Binding Isotherms" in eds. M. Yan, O. Ramstrom, Marcel Dekker, New York, N. Y., **2005**, *Molecularly Imprinted Materials*, pp. 419-434.
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G. T. Rushton, C. L. Karns, K. D. Shimizu. "A critical examination of the use of the Freundlich isotherm in characterizing molecularly imprinted polymers (MLPs)" *Anal. Chim. Acta*, **2005**, 528, 107-113.

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N. T. Greene, S. L. Morgan, K. D. Shimizu. "*Molecularly imprinted polymer sensor arrays*" *Chem. Commun.*, **2004**, 10, 1172-1173.

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M. Rampey, R. J. Umpleby, G. T. Rushton, J. C. Iseman, R. N. Shah, K. D. Shimizu. "Characterization of the imprint effect and the influence of imprinting conditions on affinity, capacity, and heterogeneity in molecularly imprinted polymers using the Freundlich isotherm-affinity distribution analysis" *Anal. Chem.*, **2004**, 76, 1123-1133.

D. L. Reger, D. M. C. Smith, K. D. Shimizu, M. D. Smith. "Syntheses and solid state structures of europium and terbium complexes of N,N'-bis(2-pyridylmethyl)urea and N,N'-bis(3-pyridylmethyl)oxalamide" *Polyhedron*, **2004**, 23, 711-717.

R. J. Umpleby, II, A. M. Rampey, S. C. Baxter, G. T. Rushton, R. N. Shah, J. C. Bradshaw, K. D. Shimizu. "Characterization of the heterogeneous binding site affinity distributions in molecularly imprinted polymers" *J. Chromatogr. B*, **2004**, 804, 141-149.

L. S. Shimizu, A. D. Hughes, M. D. Smith, M. J. Davis, B. P. Zhang, H. C. zur Loye, K. D. Shimizu. "*Self-assembled nanotubes that reversibly bind acetic acid guests*" *J. Am. Chem. Soc.*, **2003**, 125, 14972-14973.

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S. Shotwell, H. L. Ricks, J. G. M. Morton, M. Laskoski, J. Fiscus, M. D. Smith, K. D. Shimizu, H. C. zur Loye, U. H. F. Bunz. "Trans-spanning acetylenic bispyridine ligands: synthesis and structural characterization of novel organic and organometallic pseudodehydroannulenes" *J. Organomet. Chem.*, **2003**, 671, 43-51.

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- Y. S. Chong, M. D. Smith, K. D. Shimizu. "A Conformationally Programmable Ligand" *J. Am. Chem. Soc.*, **2001**, 123, 7463-7464.
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