

DR. DARRIN J BELLETT, ASSOCIATE PROFESSOR OF CHEMISTRY

Department of Chemistry and Biochemistry, Baylor University, One Bear Place #97348, Waco, TX 76798
Darrin_Bellert@baylor.edu (254)710-6863

RESEARCH PROGRAM OVERVIEW

The Bellert group researches ion/molecule reactions powered by the absorption of a single visible photon. Such systems model photo-catalysis where a transition metal converts the energy of a visible photon into the energy that powers chemical transformations. Photo-catalysis is studied by measuring the decomposition kinetics and dynamics of a photon-driven, metal mediated decomposition reaction of an organic molecule. The role of the transition metal is two-fold: (i) to act as a chromophore absorbing the visible photon and depositing this quantum of energy into the reaction coordinate, and (ii) to act as a catalytic active site by reducing the energy requirements to rearrange and break the covalent bonds between the atoms of an organic molecule. This research is novel, and we have developed custom instrumentation to measure the microcanonical decomposition kinetics and dynamics of metal mediated reactions.

CURRENT FUNDING

ACS PRF \$110,000. Funding period 09/01/18 to 08/31/2020
Earth Abundant Transition Metal Oxides and Carbides as Super-Atom Molecular Analogs to Platinum.

PROFESSIONAL PREPARATION

- Wright State University, Dayton, OH
Bachelor of Science, Chemistry, 1986 – 1992
- University of Florida, Gainesville, FL
Doctor of Philosophy, Physical Chemistry, 1992 – 1998
Ph. D. mentor: Professor Phillip Brucat
Dissertation: *Solute-Solvent Interactions of Transition Metal Containing Complexes Determined via Gas-Phase Photodissociation Spectroscopy*
- University of Utah, Salt Lake City, UT
Post-doctoral fellow, Assistant Research Professor, 1998 - 2003
Mentor: Professor Bill Breckenridge
- Baylor University, Waco, TX
Assistant Professor of Chemistry, 2003 – 2009
Associate Professor of Chemistry, 2009 – 2019

PERSONNEL

<i>Ph. D. Student</i>	<i>Graduation Year</i>	<i>Position</i>
Jason Dee	2010	University of Texas at Austin, laboratory coordinator
Vanessa Castleberry	2010	Baylor University, senior lecturer
Otsmar Villarroel	2012	McLennan Community College, senior lecturer
Ivanna Laboren	2012	McLennan Community College, senior lecturer
Adam Mansell	2016	University of Florida, undergraduate research director
Zachary Theis	2019	Air Force Research Laboratory, Civilian Scientist
Michael Gutierrez	2019	Harding University, Assistant Professor
Tucker Lewis	2021	Graduate researcher, Baylor University

LIST OF SCIENTIFIC PUBLICATIONS
BY
DARRIN J. BELLERT, PH. D.

- 1 Z. Theis, M. G. Gutierrez, T. W. R. Lewis, A. Mansell, O. N. Faza, E. Mastin, C. Silva López, and D. J. Bellert, Rate-Limiting Hydrogen Transfers in the Ni⁺ Mediated Decomposition of Diethyl Ether, *PCCP*, 2019, article under review.
- 2 M. G. Gutierrez, Z. Theis, T. W. R. Lewis and D. J. Bellert, A molecular beam apparatus for performing single photon initiated dissociative rearrangement reactions (SPIDRR) with transition metal cation bound organic clusters, *Rev. Sci. Instrum.*, **89**, 074101, 2018, DOI:10.1063/1.5024939.
- 3 A. Mansell, D. Kahle and D. J. Bellert, Calculating RRKM Rate Constants from Vibrational Frequencies and Their Dynamic Interpretation, *Math. J.*, **19**, 2017 DOI:10.3888/tmj.19-5.
- 4 C. Silva López, O. N. Faza, A. Mansell, Z. Theis and D. Bellert, Three Reaction Channels with Signature Proton Transfers in the Ni(I)-Catalyzed Decomposition of Ethyl Acetate, *Organometallics*, 2017, **36**, 761–766, DOI: 10.1021/acs.organomet.6b00769.
- 5 A. Mansell, Z. Theis, M. G. Gutierrez, O. N. Faza, C. S. Lopez and D. J. Bellert, Submerged Barriers in the Ni⁺ Assisted Decomposition of Propionaldehyde, *J. Phys. Chem. A*, 2016, **120**, 2275–2284, DOI: 10.1021/acs.jpca.5b08444.
- 6 N. A. Van Der Velde, H. T. Korbitz, D. J. Bellert and C. M. Garner, Kinetic Studies of the Epimerization of Diastereomeric Pyrylium Salts, *J. Org. Chem.*, 2013, **78**, 11698–11706, DOI: 10.1021/jo401620w.
- 7 O. J. Villarroel, I. E. Laboren and D. J. Bellert, Co⁺-Assisted Decomposition of h₆ - Acetone and d₆ - Acetone: Acquisition of Reaction Rate Constants and Dynamics of the Dissociative Mechanism, *J. Phys. Chem. A*, 2012, **116**, 3081–3088, DOI:10.1021/jp2047135.
- 8 I. E. Laboren, O. J. Villarroel, S. J. Dee, V. A. Castleberry, K. Klausmeyer and D. J. Bellert, Reaction Rate Constants and Mechanistic Detail of the Ni⁺ + Butanone Reaction, *J. Phys. Chem. A*, 2011, **115**, 1810–1820, DOI: 10.1021/jp111487r.
- 9 S. J. Dee, V. A. Castleberry, O. J. Villarroel, I. E. Laboren and D. J. Bellert, Low-Energy Reaction Rate Constants for the Ni⁺ -Assisted Decomposition of Acetaldehyde: Observation of C–H and C–C Activation, *J. Phys. Chem. A*, 2010, **114**, 1783–1789, DOI: 10.1021/jp910396t.
- 10 S. J. Dee, V. A. Castleberry, O. J. Villarroel, I. E. Laboren, S. E. Frey, D. Ashley and D. J. Bellert, Rate-Limiting Step in the Low-Energy Unimolecular Decomposition Reaction of Ni⁺• Acetone into Ni⁺CO + Ethane, *J. Phys. Chem. A*, 2009, **113**, 14074–14080, DOI: 10.1021/jp906912d.
- 11 V. A. Castleberry, S. Jason Dee, O. J. Villarroel, I. E. Laboren, S. E. Frey and D. J. Bellert, The Low-Energy Unimolecular Reaction Rate Constants for the Gas Phase, Ni⁺-Mediated Dissociation of the C–C σ Bond in Acetone, *J. Phys. Chem. A*, 2009, **113**, 10417–10424, DOI: 10.1021/jp904561y.
- 12 V. Castleberry, J. Dee, O. Villarroel, I. Laboren and D. Bellert, Two Photon Resonant Excitation

- of Copper–Rydberg levels, *Phys. Lett. A*, 2008, **372**, 4805–4808, DOI: 10.1016/j.physleta.2008.04.059.
- 13 S. O. Fakayode, M. A. Busch, D. J. Bellert, and K. W. Busch, Determination of the Enantiomeric Composition of Phenylalanine Samples by Chemometric Analysis of the Fluorescence Spectra of Cyclodextrin Guest–Host Complexes, *Analyst*, 2005, **130**, 233–241.
 - 14 J. Wang, N.-T. Van-Oanh, D. Bellert, W. H. Breckenridge, M. A. Gaveau, E. Gloaguen, B. Soep and J. M. Mestdagh, Laser spectroscopic studies of the $E^1\Sigma^+$ ‘Rydberg’ state of the MgO molecule, *Chem. Phys. Lett.*, 2004, **392**, 62–67.
 - 15 D. Bellert, K. L. Burns, N. T. Van-Oanh, J. Wang and W. H. Breckenridge, Spectroscopic characterization of the $F^1\Pi_1$ ‘Rydberg’ state of the MgO molecule, *Chem. Phys. Lett.*, 2003, **381**, 725–728.
 - 16 D. Bellert, K. L. Burns, N. T. Van-Oanh, J. Wang and W. H. Breckenridge, A new source for vibrationally excited and rotationally cold metal-oxide molecules: spectroscopic characterization of the low-lying $a^3\Pi_2$ metastable excited state of the MgO molecule, *Chem. Phys. Lett.*, 2003, **381**, 381–384.
 - 17 D. Bellert, D. K. Winn and W. H. Breckenridge, Spectroscopic Characterization of the First Singlet (\tilde{A}^1B_1) Excited State of $^7\text{Li}^{16}\text{O}^7\text{Li}$, *J. Chem. Phys.*, 2003, **119**, 10169–10174.
 - 18 D. Bellert, D. K. Winn and W. H. Breckenridge, Rovibrational Energy Levels of the LiOLi Molecule from Dispersed Fluorescence and Stimulated Emission Pumping Studies, *J. Chem. Phys.*, 2002, **117**, 3139–3148.
 - 19 D. J. Bellert and W. H. Breckenridge, Bonding in Ground-State and Excited-State $A^+\text{Rg}$ van der Waals Ions ($A = \text{Atom}$, $\text{Rg} = \text{Rare-Gas Atom}$): A Model-Potential Analysis, *Chem. Rev.*, 2002, **102**, 1595–622
 - 20 D. Bellert, D. K. Winn, and W. H. Breckenridge, Spectroscopic Determination of the Vibrational Frequencies of the First 1B_1 Excited State of LiOLi, *Chem. Phys. Lett.*, 2002, **355**, 151–158.
 - 21 D. Bellert, D. K. Winn, and W. H. Breckenridge, Dispersed Fluorescence Studies of Linear LiOLi: a Strongly Bound, but Very ‘Floppy’ Ionic Molecule, *Chem. Phys. Lett.*, 2001, **348**, 39–46.
 - 22 D. Bellert and W. H. Breckenridge, A resonant Two-Color Photoionization Threshold Determination of the Ionization Energy of the LiOLi Molecule, *Chem. Phys. Lett.*, 2001, **337**, 103–106.
 - 23 K. L. Burns, D. Bellert, A. W. K. Leung and W. H. Breckenridge, M^+/Rg bonding: The Effects of M^+ Permanent Quadrupole Moments ($M^+ = \text{Atomic Metal Ion}$; $\text{Rg} = \text{Rare Gas Atom}$), *J. Chem. Phys.*, 2001, **114**, 7877–7885.
 - 24 D. Bellert and W. H. Breckenridge, A Spectroscopic Determination of the Bond Length of the LiOLi Molecule: Strong Ionic Bonding, *J. Chem. Phys.*, 2001, **114**, 2871–2874.
 - 25 K. L. Burns, D. Bellert, A. W. K. Leung and W. H. Breckenridge, The Effects of Dispersive

- C_n/R_n -attraction on M^+/Rg bonding (M^+ =atomic metal ion, Rg =rare gas atom), *J. Chem. Phys.*, 2001, **114**, 2996–3002.
- 26 D. Bellert, K. L. Burns, R. Wampler, and W. H. Breckenridge, An Accurate Determination of the Ionization Energy of the MgO Molecule, *Chem. Phys. Lett.*, 2000, **322**, 41–44.
- 27 A. W. K. Leung, D. Bellert, and W. H. Breckenridge, Spectroscopic Analysis of an Unusual $Ca \cdot Xe[{}^3\Sigma^-] \leftarrow Ca(4s4p\pi^3P_0) \cdot Xe[{}^3\Pi_0^-]$ transition, *J. Chem. Phys.*, 1999, **111**, 6434–6438.
- 28 A. W. K. Leung, J. G. Kaup, D. Bellert, J. G. McCaffrey, and W. H. Breckenridge, Spectroscopic Characterization of the Weakly Bound $Ca(4s4d\sigma^3D_3) \cdot Ar[{}^3\Sigma^+]$ State: Evidence for a Substantial Maximum in the Potential Curve at Long Range, *J. Chem. Phys.*, 1999, **111**, 2484–2489.
- 29 A. W. K. Leung, J. G. Kaup, D. Bellert, J. G. McCaffrey and W. H. Breckenridge, Spectroscopic Characterization of Excited $Ca(4s4d\delta^3D_1)RG({}^3\Delta_{1,2})$ states ($RG=Ar, Kr, Xe$): No “Heavy-Atom” Mixing of $RG(nd\delta)$ character into the Wave Functions, *J. Chem. Phys.*, 1999, **111**, 981–987.
- 30 J. G. McCaffrey, D. Bellert, A. W. K. Leung, and W. H. Breckenridge, Spectroscopic Characterization of the $Zn(4s^2) \cdot Ne[{}^1\Sigma^+]$ and $Zn(4s4p\pi) \cdot Ne[{}^1\Pi_1]$ van der Waals States, *Chem. Phys. Lett.*, 1999, **302**, 113–118.
- 31 A. W. K. Leung, D. Bellert, R. R. Julian, and W. H. Breckenridge, Resonant Two-Color Photoionization Threshold Measurements of the $Zn^+(4s) \cdot Ar$ Bond Strength: Model-potential Analysis of $M^+(ns) \cdot Ar$ Interactions, *J. Chem. Phys.*, 1999, **110**, 6298–6305.
- 32 A. Kamariotis, T. Hayes, D. Bellert, and P. J. Brucat, The Ground and Charge-Transfer Excited States of CoO^+ , *Chem. Phys. Lett.*, 2000, **316**, 60–66.
- 33 D. Bellert, T. Buthelezi and P. J. Brucat, The structure of $Co^+ \bullet OCO$, *Chem. Phys. Lett.*, 1998, **290**, 316–322.
- 34 T. Hayes, D. Bellert, T. Buthelezi and P. J. Brucat, The bond length of VAr^+ , *Chem. Phys. Lett.*, 1998, **287**, 22–28.
- 35 D. Bellert, T. Buthelezi, T. Hayes and P. J. Brucat, The gas-phase solvation of the zirconium oxide ion: $ZrO^+ \bullet CO_2$ and $ZrO^+ \bullet N_2$, *Chem. Phys. Lett.*, 1997, **276**, 242–249.
- 36 D. Bellert, T. Buthelezi, T. Hayes and P. J. Brucat, The binding energy and vibronic structure of $NbXe^+$, *Chem. Phys. Lett.*, 1997, **277**, 27–32.
- 37 T. Hayes, D. Bellert, T. Buthelezi and P. J. Brucat, The photodissociation of $V^+ \bullet CH_4$, *Chem. Phys. Lett.*, 1997, **264**, 220–224.
- 38 T. Buthelezi, D. Bellert, T. Hayes and P. J. Brucat, The adiabatic binding energy of $NbAr^+$, *Chem. Phys. Lett.*, 1996, **262**, 303–307.
- 39 D. Bellert, T. Buthelezi, K. Dezfulian, T. Hayes and P. J. Brucat, The binding energy of VXe^+ , *Chem. Phys. Lett.*, 1996, **260**, 458–464.
- 40 T. Buthelezi, D. Bellert, V. Lewis, K. Dezfulian, J. Kisko, T. Hayes and P. J. Brucat, Vibronic

transitions in Ni_2^+ , *Chem. Phys. Lett.*, 1996, **257**, 340–346.

- 41 D. Bellert, T. Buthelezi, V. Lewis, K. Dezfulian, D. Reed, T. Hayes and P. J. Brucat, The rovibronic structure of Ni_2^+ via resonant two-color photodissociation, *Chem. Phys. Lett.*, 1996, **256**, 555–560.
- 42 T. Buthelezi, D. Bellert, V. Lewis and P. J. Brucat, The C←X transition in CaKr^+ and CaAr^+ , *Chem. Phys. Lett.*, 1995, **246**, 145–149.
- 43 T. Buthelezi, D. Bellert, V. Lewis and P. J. Brucat, The bond length of CoKr^+ , *Chem. Phys. Lett.*, 1995, **242**, 627–631.
- 44 D. Bellert, T. Buthelezi, V. Lewis, K. Dezfulian and P. J. Brucat, Reply to the Comment on “The binding energy of $\text{Ni}^+\bullet(\text{N}_2\text{O})$ ”, *Chem. Phys. Lett.*, 1995, **247**, 614–615.
- 45 D. Bellert, T. Buthelezi, V. Lewis, K. Dezfulian and P. J. Brucat, The binding energy of $\text{Ni}^+\bullet(\text{N}_2\text{O})$, *Chem. Phys. Lett.*, 1995, **240**, 495–498.
- 46 R. L. Asher, D. Bellert, T. Buthelezi, V. Lewis and P. J. Brucat, A measure of the effective electric-dipole polarizability of argon, *Chem. Phys. Lett.*, 1995, **234**, 113–118.
- 47 R. L. Asher, D. Bellert, T. Buthelezi, D. Lessen and P. J. Brucat, The bond length of ZrAr^+ , *Chem. Phys. Lett.*, 1995, **234**, 119–122.
- 48 R. L. Asher, D. Bellert, T. Buthelezi and P. J. Brucat, Optical Excitation of $\text{Co}^+\bullet\text{N}_2$, *J. Phys. Chem.*, 1995, **99**, 1068–1072.
- 49 R. L. Asher, D. Bellert, T. Buthelezi, G. Weerasekera and P. J. Brucat, The binding energy of $\text{Ni}^+\bullet\text{CO}_2$, *Chem. Phys. Lett.*, 1994, **228**, 390–392.
- 50 R. L. Asher, D. Bellert, T. Buthelezi and P. J. Brucat, Spin forbidden transitions in NiAr^+ , *Chem. Phys. Lett.*, 1994, **228**, 599–604.
- 51 R. L. Asher, D. Bellert, T. Buthelezi and P. J. Brucat, The $\text{Co}^+\bullet\text{CO}_2$ electrostatic complex: Geometry and potential, *Chem. Phys. Lett.*, 1994, **227**, 623–627.
- 52 R. L. Asher, D. Bellert, T. Buthelezi and P. J. Brucat, The ground state of CoAr^+ , *Chem. Phys. Lett.*, 1994, **227**, 277–282.
- 53 R. L. Asher, D. Bellert, T. Buthelezi and P. J. Brucat, The bond strength of Ni_2^+ , *Chem. Phys. Lett.*, 1994, **224**, 529–532.
- 54 R. L. Asher, D. Bellert, T. Buthelezi and P. J. Brucat, The bond length of Ni_2^+ , *Chem. Phys. Lett.*, 1994, **224**, 525–528.