The Department of Chemistry,
Department of Physics & Astronomy,
Cain Department of Chemical Engineering,
and the LSU Graduate School

a celebration of the contributions of the

Coates Family

9:00 am, Thursday, March 16, 2017
French House, Grand Salon
Louisiana State University

PROGRAM
FRENCH HOUSE GRAND SALON

Session Chair:	Professor Carol M. Taylor Department of Chemistry
9:00 am	Opening Remarks: Dean Michelle Massé Graduate School
9:10 am	Ms Bijeta Prasai McCarley Group, Department of Chemistry *Fluorescent Probe Interrogation of a Cytoprotective Cancer-Linked Oxidoreductase in Two-Dimensional Human Cell Cultures and Solid Tumor Mimics*
9:30 am	Dean Cynthia B. Peterson *A Culture of Philanthropy for LSU*
10:00 am	***Coffee Break***
10:20 am	Ms Eva Caspary Wornat Group, Cain Department of Chemical Engineering *The Formation of Polycyclic Aromatic Hydrocarbons From the Pyrolysis of Model Alkene Fuels*
10:40 am	Mr Kundan Kadam Deibel Group, Department of Physics *Simulating Stellar Mergers*
11:00 am	Associate Professor Donghui Zhang Department of Chemistry *A Journey into the World of Peptidomimetic Polymers: Twists, Turns and Discovery*

POSTER SESSION
CHEMISTRY AND MATERIALS BUILDING LOBBY

12:00 pm

Ms Yuxin Fang
Flake Group, Cain Department of Chemical Engineering
Electrochemical CO_2 Reduction on Thiolated Au

Ms Elizabeth Hurst
Wornat Group, Cain Department of Chemical Engineering
Effects of Temperature on Products from the Supercritical Pyrolysis of a Model Alkene Fuel

Mr Raju Kumal
Haber Group, Department of Chemistry
Molecular Diffusion and Photothermal Kinetics Studied by Second Harmonic Generation

Ms Tyrslai Williams
Vicente Group, Department of Chemistry
Contemporary Synthesis and Investigation of Peptidic-BODIPY Conjugates

Mr Nicolas Cannady
Cherry Group, Department of Physics
Gamma-Ray Observations with the CALorimetric Electron Telescope (CALET)

Ms Amber Lauer
Deibel Group, Department of Physics
Proton Scattering on 37K

Charles E. Coates (1866-1939)

Charles Edward Coates was born in Baltimore, MD. He attended John Hopkins University, received a BA and then began graduate studies in Chemistry with Ira Remsen. His dissertation was on sulfobenzoic acid, a starting material for the synthesis of saccharin - perhaps a prophetic precursor to his career in sugar chemistry. He spent two years in Germany and completed his Ph.D. in 1891.

He came to LSU in 1893 as only the third faculty member with a Ph.D. and was assigned space in a blacksmith's shop that had been condemned by the US government. He transformed the laboratory and created a new era in chemical education at LSU. He also became the University's first football coach.

Coates is quoted as saying, "Chemistry is just as pure when applied to the solution of a problem touching the welfare of mankind as when applied merely to intellectual attractions." He had a particular commitment to Louisiana Agriculture. When the Audubon Sugar School moved to LSU in 1897, Coates was the obvious choice to lead it. The School attracted students from around the globe and the program is viewed by the some as the progenitor of Chemical Engineering education in the USA.

With the reorganization of the University in 1908, Coates became Dean of the Audubon Sugar School and Head of Chemistry, positions he held until his retirement in 1937. For 23 years he was Chairman of the Division of Graduate Studies. However, he forwent becoming Dean of the Graduate School to serve as Dean of the College of Pure and Applied Science. Coates campaigned relentlessly for better facilities and chemical literature. When LSU moved to its current location in 1926, the new Chemistry building was named Charles E. Coates Hall. The first Ph.D. at LSU was awarded to one of Coates' students in what would have been considered Chemical Engineering. Chemical Engineering became a separate department upon reorganization following Coates' retirement. Coates' son Jesse became the first Chair of Chemical Engineering.

In his personal life, Charles E. Coates married Ollie Maurin in 1901 and they had four children: Charles Hunter, Victor Maurin, Jesse and Caroline Pennock.

A nephew of Coates, George Hunter Coates, was a student at LSU and lived with his aunt and uncle in Baton Rouge. He graduated in 1918 and went on to found Coates Energy. In gratitude to his uncle, George Coates established the Dr Charles E. Coates Memorial Fund at LSU that supports graduate student research and travel to this day.

Reference: a lecture delivered by Professor James G. Traynham to the HIST Division of the ACS in 1996, in turn extracted from documents of the Coates Family.

9:10am Bijeta Prasai, Department of Chemistry

Fluorescent Probe Interrogation of a Cytoprotective Cancer-linked Oxidoreductase in Two-dimensional Human Cell Cultures and Solid Tumor Mimics

Fluorescence molecular imaging is an emerging field with the potential to aid in optically guided surgery for cancer treatment. To overcome the drawbacks of always-fluorescent imaging probes, activatable probes, whose fluorescence can be turned on by a cancer-linked target, are being developed so as to achieve high signal-to-background imaging for better discrimination of cancer cells from normal cells. For activation, turn-on fluorescent probes rely on the presence of biomarkers that are highly specific to tumor cells. Overexpressed hNQO1 enzyme in solid tumors, a prime cancer-associated biomarker, is targeted in the McCarley Research Lab in the development of activatable molecular probes. The goal of our work is to use one such molecular probe as an hNQO1 sensor to evaluate the distribution and functionality of the enzyme in micro-regions of multicellular tumor spheroids (MCTSs) that mimic solid tumors. The ability to examine for possible spatially dependent enzyme activity in tumors is of great value in the development of imaging and chemotherapeutic agents that are activated by hNQO1.

Originally from Nepal, Bijeta Prasai came to the United States in 2008 and enrolled in Nicholls State University with Chemistry/Pre-med as her major. In the summer of 2011, the LSU LBRN program offered her an internship opportunity. This brief research experience essentially fostered her interest in research as a career. Therefore, after completing her bachelor's degree, She joined the Louisiana State University Chemistry graduate program in 2012 and has been working towards her doctoral degree under the mentorship of Professor Robin McCarley. She will graduate in August of 2017.

Bijeta was awarded the Coates travel award in 2014, which she used to attend a very prestigious Gordon Research Conference. The award gave her an opportunity to present her research before a highly specialized scientific community and to improve my communication skills. Well-known scientists in the field of biosensor from all over the states gave talks in a series of technical session, which allowed Bijeta to gain valuable insights about the recent findings made in the field both related and unrelated to her work.

9:30 am Dean Cynthia Peterson, College of Science

A Culture of Phlanthropy for LSU

Cynthia B. Peterson, a protein biochemist and LSU alumna, earned a B.S. in Biochemistry followed by a Ph.D. in Biochemistry from the LSU Health Sciences Center. She then pursued postdoctoral training at the University of California, Berkeley before assuming an assistant professor position at the University of Tennessee (UT) in 1992. Peterson was promoted to associate professor with tenure in 1997 and then to full professor in 2002. She held the Kenneth and Blaire Mossman Professorship in Biomedicine at UT and served as the Associate Dean of Academic Personnel in the College of Arts and Sciences. Peterson was appointed Dean of the College of Science at LSU in August 2014 and holds the Seola Arnaud and Richard Vernon Edwards Professorship.

Dean Cynthia Peterson serves as the Chief Executive Officer of the LSU College of Science. The College is comprised of five academic departments (Biological Sciences, Chemistry, Geology & Geophysics, Mathematics, Physics & Astronomy), the LSU Museum of Natural Sciences, and the LSU Herbarium. Dean Peterson is responsible for all aspects of academic life within the College, including teaching, research, and budgetary matters. She formulates and administers policies for the College and sets priorities through the development of the College's Strategic Plan. Dean Peterson leads all fund raising activities for the College, seeking charitable gifts for endowed chairs and the creation or restoration of facilities. She is responsible for all personnel matters within the College and coordinates with departments to identify focus areas for new faculty hires and set salaries and startup packages. The College of Science also has active collaborations with several federally funded interdisciplinary programs and facilities, such as LIGO, funded by the National Science Foundation, the Louisiana Consortium for Neutron Scattering, funded by the US Department of Energy, and the Louisiana Space Consortium, funded by NASA. The College provides leadership for the Center for Advanced Microstructures and Devices (CAMD), one of seven synchrotron facilities in the United States. The College also provides numerous unique learning opportunities for students through several Research Experience for Undergraduates (REU) programs in various disciplines and the LSU Geology Field Camp in Colorado Springs, Colorado.

10:20am Eva Caspary, Cain Department of Chemical Engineering

The Formation of Polycyclic Aromatic Hydrocarbons From the Pyrolysis of Model Alkene Fuels

To understand the role of 1-alkenes and allylic radicals in the reaction pathways leading to the formation and growth of polycyclic aromatic hydrocarbons (PAH), pyrolysis experiments have been performed with three different 1-alkene fuels: propylene, 1-butene, and 1-pentene. Each of these fuels has been pyrolyzed at temperatures of 600 – 1000 °C and a fixed residence time of 0.31 s. The experiments are carried out in an isothermal laminar-flow quartz-tube reactor and the pyrolysis products are analyzed by gas chromatography with flame-ionization detection and thermal-conductivity detection, for $C_1 - C_6$ hydrocarbon products and H_2; gas chromatography with flame-ionization detection and mass-spectrometric detection, for one- and two-ring aromatic hydrocarbon products; and high-pressure liquid chromatography with ultraviolet-visible absorbance detection, for PAH products ≥ 3 rings. The identities and temperature-dependent product yields of propylene pyrolysis, 1-butene pyrolysis, and 1-pentene pyrolysis will be presented and discussed.

Eva Caspary obtained her Bachelor's in Process Engineering from the University of Applied Sciences in Mannheim, Germany in the year 2009. Currently, she is pursuing her Ph.D. in Chemical Engineering at LSU under Professor Mary J. Wornat. During the time of her doctoral studies, Eva Caspary has co-authored one peer-reviewed journal article and has had the chance to give seven conference and poster presentations at various meetings in America, Europe, and Asia. Eva's research deals with understanding the formation pathways of polycyclic aromatic hydrocarbons (PAH) from the pyrolysis of solid, liquid, and gaseous fuels. She anticipates receiving her doctoral degree in Spring 2017.

Eva has received the Coates Travel Award to assist with travel cost to two different conferences: the 25th International Symposium on Polycyclic Aromatic Compounds held in Bordeaux, France in September 2015 and the 36th International Symposium on Combustion held in Seoul, South Korea in August 2016. At both meetings, she has had the invaluable opportunity to present her work, to network with many world-renowned scientists, and to represent LSU as a high-profile research university.

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10:40am Kundan Kadam, Department of Physics

Simulating Stellar Mergers

Binary stellar systems are immensely important for our understanding of the universe as well as various astronomical phenomena. A contact binary is a type of binary system, where the two stars are so close that they touch each other, while revolving around their center of mass. My dissertation was inspired by a particular observed event that occurred in 2008, called V1309 Sco. This type of event is known as Luminous Red Nova, and in this case it turned out to be the result of the merger of a contact binary system. The final eruption was shown to be the disruption of the core of the secondary inside the more massive star. I study dynamical mass transfers and mergers of close and contact binary systems through extensive numerical modeling and hydrodynamic simulations. This is the first attempt in the astrophysics community to simulate binary systems where both the components have bipolytropic equation of state, with a fully resolved core and envelope structure.

Kundan Kadam was born in Bombay, India, on December 4th 1984. He was raised in India and obtained both his Bachelor and Master of Science degrees from the University of Mumbai. From year 2009 to present, he attended the Graduate Program in Physics at the Louisiana State University, Baton Rouge. Kundan expects to receive his doctorate degree in May of 2017.

The Coates Travel Awards has helped Kundan immensely while traveling for research purposes. He received the Coates award in 2013, which allowed him to travel to NuGrid collaboration meeting in Victoria, BC. Kundan also attended his first two American Astronomical Society meetings in 2014 and 2015 through the Coates Travel Award, which enabled him to present his research work.

11:00am Donghui Zhang, Department of Chemistry

A Journey into the World of Peptidomimetic Polymers: Twist and Turns and Discovery

Peptidomimetic polymers broadly refer a class of polymers whose molecular structures are similar to those of polypeptides. They emulate polypeptides in their ability to fold into higher order structures. Previous studies have shown that these polymers are backbone degradable, often biocompatible and in some cases thermally processable. Polypeptoids, a.k.a. poly(N-substituted glycine)s, do not have stereogenic centers and hydrogen bonds along the main chains, due to the N-substitution, in contrast to polypeptides. This makes the physicochemical properties of the polypeptoids strongly dependent on the side chain substituents, allowing for tuning of the polymer conformation, solubility, crystallinity, hydrophilicity-lipophilicity balance (HLB) and charge characteristic by adjusting the sidechain structure. I will present our research efforts in the development of controlled polymerization methods towards well-defined polypeptoids and polypeptides and giving examples to showcase the application of our chemistry in the development of functional biomaterials for targeted biomedical applications.

Donghui Zhang is an Associate Professor of Chemistry at the Louisiana State University. She obtained her B.S. in Chemistry from Peking University in 1998 and Ph.D. in Organometallic Chemistry from Dartmouth College in 2003 and did one and a half year of postdoctoral research at the University of Minnesota on the synthesis and characterization of polymers from biorenewable source materials. She joined LSU in 2007 after a two-year stint as a research assistant professor at New Mexico State University. Her research interests include polymer catalysis, synthesis and characterization of biomimetic, bioinspired and bio-relevant functional polymers, high precision macromolecules.

Poster: Yuxin Fan, Cain Department of Chemical Engineering

Electrochemical CO_2 Reduction on Thiolated Au

Electrochemical reduction of CO_2 can potentially play a prominent role in the development of a sustainable energy and material infrastructure for the future: It can be used as an energy carrier (including in energy-dense, transportation-ready forms) to store energy from intermittent, distributed sources such as wind and the sun. It can also be used as a renewable source of carbon for chemical production. The key to enable this greenhouse gas to fuel process is to maximize the energy efficiency of electrochemical CO_2 reduction. In present work, we will demonstrate how we can affect the efficiency with thiol ligand functionalized Au cathode electrode.

Yuxin Fang was born in Shanghai, China. She did her first 2 years of undergraduate study in Material Science at East China University of Science and Technology; and the last 2 years in Chemical Engineering at University of Missouri, Columbia. Currently, She is a 4th year graduate student in Chemical Engineering supervised by Dr. John Flake. Her research focuses on designing the energy-efficient cathode electrocatalyst for electrochemical CO_2 reduction. Yuxin is expecting to graduate in Fall 2017/Spring 2018.

In fall 2016, Yuxin received the Coates travel award for the oral presentation on “Tuning the Selectivity of CO2 Electrochemical Reduction Toward Hydrocarbon with Ligand Modified Metal Electrocatalyst” at the 230th Electrochemistry Society Conference in Hawaii. Attending this prime meeting provided her a great chance to interact with researchers in the community and get inspired by the shared knowledge.

Poster: Elizabeth Hurst, Cain Department of Engineering

Effects of Temperature on Products from the Supercritical Pyrolysis of a Model Alkene Fuel

In order to investigate the role 1-alkenes have in the formation and growth of polycyclic aromatic hydrocarbons (PAH) in the precombustion environment of future hypersonic aircrafts, supercritical pyrolysis experiments have been performed with model fuel 1-octene, a representative 1-alkene product of supercritical n-alkane fuel pyrolysis. The experiments are conducted in an isothermal silica-lined stainless steel tubular reactor at a constant pressure of 94.6 atm, a fixed residence time of 133 sec, and at five temperatures ranging from 450 to 535 °C. The PAH products, a highly complex mixture of unsubstituted and alkylated PAH, are separated using a two-dimensional chromatographic technique and are analyzed by ultraviolet-visible diode-array detection and mass spectrometry. The effects of temperature on the yields of the products from the supercritical 1-octene pyrolysis experiments will be presented, and the mechanisms of 1-octene decomposition and PAH formation and growth will be discussed.

Elizabeth Hurst received her Bachelor's degree in Chemical Engineering from Tulane University in May 2013. She joined the graduate chemical engineering program at LSU in August 2013 and is pursuing a Ph.D. under Prof. Mary J. Wornat. In spring 2016, she received the Donald W. Clayton Ph.D. Graduate Assistantship. Currently, she studies the formation and growth reactions of polycyclic aromatic hydrocarbons (PAH) from the supercritical pyrolysis of jet fuels. Elizabeth has co-authored a paper in a peer-reviewed journal and has presented two posters and given one talk at international conferences in the United States, South Korea, and France.

Elizabeth was a recipient of the Coates Travel Award, and this award helped support her travels to Seoul, South Korea where she attended the 36th International Symposium on Combustion in August 2016. At this conference, she was able to present a poster on her research while getting the opportunity to represent LSU and connect with many young researchers and prestigious scientists from around the world.

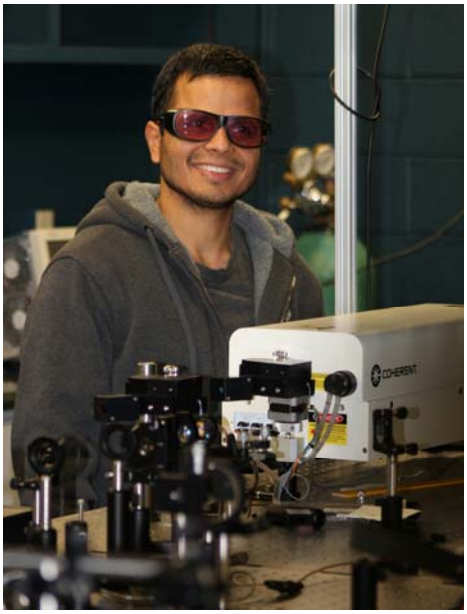
Poster: Raju Kumal, Department of Chemistry

Molecular Diffusion and Photothermal Kinetics Studied by Second Harmonic Generation

Second harmonic generation (SHG) is used to investigate molecular adsorption and diffusion kinetics of positively charged dyes at the surface of liposomes in water. The adsorption and time-dependent SHG results are analyzed to obtain the free energies of adsorption, the adsorption site densities, and the diffusion kinetics under varying liposome chemistries and buffer conditions. Parameters such as electrostatic interactions, the chemical structure of the lipid head group, the buffer conductivity, ion-pair formation and adsorbate-adsorbate repulsion are found to influence the adsorption and diffusion at the liposome surface. Additionally, gold-silver-gold core-shell-shell nanoparticles are prepared and are functionalized with miRNA using Diels-Alder chemistry. Photothermal release of oligonucleotides from the nanoparticle surface under NIR irradiation is studied for drug-delivery applications in the NIR optical window of biological tissue. Additional characterization methods such as transmission electron microscopy, electrophoretic mobility, fluorimetry, and extinction spectroscopy are used to verify the SHG results. Real-time SHG measurements are shown to be highly sensitive for investigating surface dynamics in nanoparticle-based drug delivery systems.

Raju Kumal is a fifth year graduate student in Professor Louis Haber's Group in the Department of Chemistry at Louisiana State University. He completed his Masters and undergraduate degree from Tribhuvan University of Nepal before moving to the United States. His research focuses on ultrafast and nonlinear spectroscopy and nanoparticle synthesis for potential applications in drug delivery, sensing, catalysis and photovoltaics. Raju received a Coates Scholar Research Award in 2016 for his work on liposome and gold-silver-gold core-shell-shell nanoparticles for designing drug delivery systems.

Raju was awarded Coates Scholar Research and Coates Travel Awards during his Ph.D. which have been very useful to promote his research career. He was able to go to the National Meeting of American Chemical Society to present his research work in front of scientific community. The Coates Scholar Research award for the liposome and gold-silver-gold core-shell-shell nanoparticle projects is helping the designi of drug delivery systems.



Poster: Tyrslai Williams, Department of Chemistry

Contemporary Synthesis and Investigation of Peptidic-BODIPY Conjugates

Epidermal Growth Factor Receptor (EGFR) is a protein found overexpressed at the cell surface of various cancerous cells, such as colorectal cancer (CRC). This overexpression occurs during binding to the endogenous ligand EGF. Detecting these cancer cells through imaging with fluorescent molecules that possess CRC selectivity is fundamental. BODIPY dyes were used due to their attractive photophysical properties. The small fluorescent compounds are easily altered and stable in various conditions. Two fluorescent BODIPY dyes were used to manifest the conjugates via Click chemistry, each with unique absorption properties. T3 and T4 are conjugates from linear peptides K(N_3)LARLLT, and one conjugate advanced from a cyclic peptide cyclo[K(N_3)LARLLT] to form conjugate T5. All clicked reactions showed percent yields over 50% as anticipated. Preliminary *in vitro* studies showed all compounds were found to have low phototoxicity making them beneficial for imaging through CRC, as well as compound T5 showing high specificity for EGFR in competitive binding studies. Further studies showed these compounds all had ideal cellular uptake, and are ideal candidates for future *in vivo* studies.

Tyrslai Menyaee' Williams was born to Ranetta E. Williams in Baton Rouge, Louisiana, where she completed her primary studies as salutatorian of her 2004 class. She completed her undergraduate degree at Southern University A&M College in May of 2011. Tyrslai found interest in public health and wanted to become a medical doctor until a professor at Southern University introduced her to the endless possibilities of pursuing a Ph.D. doctoral program. In August of 2011, she enrolled in Louisiana State University to obtain her Doctor of Philosophy degree in organic chemistry under the direction of Professor Graça H. Vicente. She will be awarded her degree at the August 2017 commencement.

The Dr. Charles E. Coates Memorial Travel Award allowed Tyrslai to share her research findings at the 9th Annual International Conference on Porphyrins and Phthalocyanines (ICPP-9) in Nanjing, China in July 2016. Tyrslai's research findings were accepted into the "BODIPY Dyes: Past, Present and Future" symposium that took place at ICPP-9 with top scholars of BODIPY chemistry from around the world. The advice she has received toward her research, positive feedback on the design of her research, and the knowledge gained during six days was invaluable, for in which she is forever grateful.

Poster: Nicholas Cannady, Department of Physics

Gamma-Ray Observations with the CALorimetric Electron Telescope (CALET)

The CALorimetric Electron Telescope (CALET) is a cosmic-ray instrument deployed to the International Space Station in October 2015. The primary instrument, CAL, is a 30 X0 calorimeter sensitive to electrons, protons and heavy nuclei, and gamma-ray events with energies ~1 GeV to ~30 TeV. The reconstruction and isolation of gamma-ray events in the CAL enables measurements of the galactic diffuse emission, of signals from known sources such as supernova remnants, and potentially of counterpart emission to gravitational wave events and gamma-ray bursts. This work details the process of reconstruction and separation of gamma-ray events and the calculation of instrument response functions for the CAL to yield fluxes and upper limits.

Nicholas Cannady is a graduate student in the Department of Physics and Astronomy pursuing a Ph.D. in particle astrophysics. He completed Bachelor's degrees in Physics and Mathematics at LSU, and is studying under Professor Michael Cherry. His thesis work utilizes the CALorimetric Electron Telescope (CALET), which was launched to the International Space Station (ISS) in October 2015. Specifically, his analysis focuses on the isolation of gamma-ray events in the calorimeter to provide observation of known gamma-ray sources and to search for potential counterpart events to gamma-ray bursts and gravitational wave detections. He lives in Baton Rouge with his partner, Laura.

Nicholas received a Coates Award in July 2015 to travel to the International Cosmic Ray Conference in The Hague, Netherlands, where he presented on the expected performance of the CALET instrument as a gamma-ray telescope based on simulated events and known ISS orbital parameters.

Poster: Amber Lauer, Department of Physics

Proton Scattering on 37K

The 34Ar(α,p)37K reaction is important in Type I X-ray bursts (XRBs), where nucleosynthesis proceeds through the α,p and rp processes up to A<100. Waiting -point nuclei in XRBs (e.g. 34Ar) are in (p,γ)-(γ,p) equilibrium and may stall the burst, but the (α,p) reaction may provide a detour. We performed 37K+p elastic scattering to study the compound nucleus 38Ca at the ReA3 facility at the National Superconducting Cyclotron Laboratory using a 37K beam incident on a CH2 target. Scattered protons were detected in telescopes of Si strip detectors, while coincident heavy recoils were detected in a gas ionization chamber. Experimental results will be presented and implications for XRB nucleosynthesis and observables discussed.

Amber Lauer studies the nuclear processes that happen in stars and relates experimental nuclear physics to the observables and unknowns in the stellar population. This involves a healthy mix of tinkering, programming, and making, and is incredibly fulfilling to her mad scientist's nature. She is a returning student who decided to pursue advanced education later in life. She loves space, stars, and science in general. She takes an active interest in diversity and equality in education, participating whenever possible in efforts to improve inclusion in STEM. She also enjoys music, singing, and crafts, and loves running.

The Coates Award Amber received helped fund her trip to the National Superconducting Cyclotron Laboratory. She was able to live on site for five weeks and participate in the successful experiment that comprised her Ph.D. work.

Charles E. Coates Hall (photo credit:Vickie Tate Thornton)

The plantation desk of Charles Edward Coates.
Donated to the Department of Chemistry by Coates' descendents in 2017.