CHEM 5533 COURSE SYLLABUS

University of Missouri – Kansas City
School of Biological Sciences and Chemistry

Course Number and Title: CHEM 5533 Quantum Chemistry
Catalog Number: 46942
Semester and Year: Fall 2019
Number of Credits: 3
Class Meetings: Online Synchronous – MW – 5:00 pm to 6:45 pm
Classroom Location: Online Synchronous via Canvas (https://online.umkc.edu/lms/)

Instructor: **Sai Siva Kumar Pinnepalli**
Department of Chemistry
203 Flarsheim Hall
5110, Rockhill Rd
Kansas City, 64110

Office Hours: Email the questions/concerns or schedule an on-campus meeting in advance for discussions. The online discussion forum available on Canvas also serves as the platform. The questions will be clarified within 1 or 2 days.

Office Phone: +1 816-517-6530

UMKC E-Mail: spthb@mail.umkc.edu (preferred method of contact)

University of Missouri – Kansas City Mission

UMKC's mission is to lead in life and health sciences; to deepen and expand strength in the visual and performing arts; to develop a professional workforce and collaborate in urban issues and education; and to create a vibrant learning and campus life experience.

Chemistry MS Program Mission

The Department of Chemistry offers the M.S. degree for a major in chemistry that is accredited by the American Chemical Society. The M.S. in Chemistry is designed to offer comprehensive preparation in all areas of chemistry through hands-on laboratory training and rigorous coursework. This degree provides a foundation for those interested in pursuing careers in the pharmaceutical, government, and academic sectors. It focuses on student transformation and lay a path towards advanced degrees, such as Ph.D. in various areas of chemistry and molecular sciences.

Catalog Information

Course Description / Attributes: Quantum Chemistry is an introductory graduate course to the principles of quantum mechanics applied to atoms and molecules. A brief outlook of fundamental theories, computational models, symmetry, group theory and spectroscopy will be dealt. It focuses on the application of quantum mechanical methods to the study of systems of chemical interest. Exact solutions and approximate methods will be discussed.

Pre-requisites / Co-Requisites: CHEM 432/5530B (Physical Chemistry II), or equivalent introduction to quantum mechanics (and relevant mathematics) at the undergraduate level. Experience of online learning technology.

Restrictions / Exclusions: None.

Course Format / Instructional Mode: Online synchronous via Canvas learning management system (LMS) from August 20 through December 15, 2019. Synchronous virtual lectures will be streamed on Canvas during the class meeting times. Attendance and class participation will be monitored for every lecture.

Course Information

Student Learning Outcomes

The following SLOs are approved and the students will be able to:

- **learn** the postulates of quantum mechanics and able to **apply** for problem solving
- **perform** various mathematical operators involved in complex calculus
- **understand** the terms and concepts discussed thought the semester
- **develop** more advanced theoretical models

The topic specific SLOs will be provided at the beginning each topic. The learners are assessed through homework and in-class exams on the basis of the stated SLOs.

Required & Recommended Materials

- *No formal text for this class.* The instructor notes will be distributed well in advanced of the class meetings. The notes are a consolidated essence from various books, and it serves as a text for this course.
- *"Quantum Chemistry"* 7th Edition, by Ira N. Levine; Pearson; ISBN: 978-0321803450
- *"Quantum Chemistry"* 2nd Edition, by Donald A. McQuarrie, University Science Books, ISBN: 978-1891389504.
- Various online web portals provide wealth of information

In addition, the learners will be encouraged to read some peer-reviewed journal articles to expand their knowledge. The access to journals will be provided via Canvas web portal or can be requested through the university library via Mobius or Scifinder.

Course Technology Requirements

The students are expected to have access to necessary computing resources either through personal equipment or from university. The university library provides the latest updated softwares whose services can be utilized. The following requirements might assist you for vibrant participation in the online class:

- Internet Explorer, Google Chrome or Mozilla Firefox for Windows/ Safari for Apple operating systems
- A headset with microphone and webcam
- Updated versions of Java, Media Player and Adobe Reader or similar features for Apple and (http://get.adobe.com/reader, http://www.java.com/en)
- High-speed broadband internet connection

Technology Support

The UMKC's Instructional Technology Services (ITS) can be utilized by calling 816-235-6700 or emailing its@umkc.edu, should you have questions with regards to technical glitches. The tech support is available during the business hours (7:00 am to 6:00 pm) from Monday through Friday. Live online chat is available through the Canvas login page on Sunday and Monday nights from 6:00 pm to 10:00 pm and on Tuesday's from 8:00 pm to 10:00 pm.

Evaluation and Grading Criteria

This will be comprised of six parts: 23% of the course grade comes from each of three exams (one per "unit" of the course), 10% from homework, 15% from a 10-15 minute student video presentation near the end of the semester on a contributor to the development of quantum chemistry, with the remaining 6% coming from attendance and in-class participation (please refer to the later sections of this syllabus). The grading scale to be used will be 90-100, A; 80-89, B; 70-79, C; 60-69, D. Furthermore, the top two possible scores in each grade category (other than "A") will be awarded a "+" sign; the bottom two possible scores in each grade category (including "A's") will receive a "-" sign. For example, a final average of 90 or 91 will receive a grade of "A-;" final averages of 88 or 89 will receive "B+."

HOMEWORK: Both "essay" questions (more qualitative in nature) and problems (more quantitative in nature) will comprise the three homework assignments for the semester, and answers to these questions will be posted on Canvas prior to the exam over the corresponding

portion of the course. The homework assignments are **due by 11:59 PM on the Friday preceding each exam**. They will be graded and returned to you via Canvas prior each exam. The students may "consult" with other students and with the instructor about any questions you might have regarding the homework—but the learners must turn in their own work.

STUDENT VIDEO PRESENTATION: Each student will select a scientist who has contributed to the field of quantum chemistry or spectroscopy from a list of researchers I will distribute, and will make a short video presentation (~10 to 15 minutes or so) on that person's background and his or her contributions to the field of quantum chemistry and/or spectroscopic topics derived from quantum concepts. These short presentations will be evaluated by the other students in the class, and by the instructor, on the following basis: superior presentation = A; very good presentation = B; good presentation = C; poor presentation = D, with pluses and minuses assigned as appropriate. A major portion of the grade will be based on demonstrated learning of the topics covered this semester.

EXAMS: Each of the three exams will cover the material discussed in class during the weeks preceding each exam. Questions will be developed based on 5 D's: discuss, derive, determine, describe and define. The first exam will be on September 25th and will cover topics from our discussions through September 16th. The second exam will be on October 30th and will cover material from our discussions from September 18th through October 21st. The third exam will be on December 12th, covering the final course topics. The question paper will be posted online a day in-advance on Canvas page. The students will have 24 hours to write, upload or submit the answers.

ATTENDANCE AND IN-CLASS PARTICIPATION: Learning chemistry involves a process of "finding out," and questioning is an integral skill throughout all of science, so one of my goals for this course is to help you develop your skills in asking (and answering) questions. Everyone will start out with 20 points in this category and will be allowed one unexcused absence during the semester. I require that each student ask at least two questions in each portion of the course; for each of the six required questions not asked, I will deduct one point from the 20. For each unexcused absence, two points will be deducted from the 20. Excused absences will be granted with documentation, however, but please get in touch with me—preferably in advance—if for any reason you have to miss a class.

Course Expectations, Policies, and Requirements for Student Conduct

Late Work Policy

Students are expected to attend all the class meetings in-time. The online login time for the class is reported and considered as the attendance. The lecture contains few questions at the end which students are expected to submit the answers immediately. All other reports/ homework/exams must be submitted online via Canvas before the 11.59 pm on the due date. Late submission will not be accepted. However, late submissions will be accepted based on the situation, prior intimation and validity of the reason or during emergencies.

Professional Dispositions

A high degree of professionalism (intellectual maturity, democratic values and attitudes - respect, sensitivity, responsibility, and cooperation) is expected from all students. The online learning environment is established to simulate the actual physical classroom to outreach the learners of distant geographic locations. The policies regarding the integrity of online learning are well-laid to protect individual's learning capabilities and freedom to express their thoughts for academic and knowledge purposes. Any learner with unprofessional or disrespectful behavior, breaking the integrity of the course will be considered as a threat for safe online learning environment. This course will strive to foster a respectful learning community. The instructor reserves the right to manage a positive learning environment and thus will not condone inappropriate conduct in the course. Generally, academic/professional misconduct by a student shall include, but not be limited to: disruption of learning activities (including inappropriate online conversation), rudeness toward the instructor or other class members, insensitivity, misrepresenting information presented in class, manipulative and negative behavior, etc.

Responsibility

Each student owns their right to learnt, express and interact in the class. Every learner is responsible for their own grades. The more time you put in the course, the more you can learn and advance. Every student is also responsible to maintain a safe and ameliorate online learning environment. Please watch a training video for online learning environments and technologies (will be posted within the first two weeks).

Calendar / Course Schedule

We will be meeting twice a week to carry out two experiments. The following table lists the tentative schedule of the course for this semester:

August 19	Introductions, policies, overview of the course and its content
August 21	Historical development of quantum chemistry
August 26	Finish historical aspects, begin quantum chemistry concepts
August 28	Finish basic concepts, start free particle and 1-D particle in a box
September 2	LABOR DAY HOLIDAY (NO CLASS MEETING)
September 4	Particle in a box model in 1-D, 2-D, and 3-D
September 9	Start the simple harmonic oscillator model
September 11	Finish the SHO model, introduce vibrational spectroscopy
(September 11	*Last day to withdraw with no record on transcript)*
September 16	Angular momentum ideas, start rigid rotor model
September 18	Introduce rotational spectroscopy, review material for EXAM I
September 23	The hydrogen atom (not on EXAM I)
September 25	EXAM I
September 30	The hydrogen atom and the Periodic Table

October 2	Finish the Periodic Table, start the hydrogen molecule ion
October 7	Valence bond theory, molecular orbital theory
October 9	Quantum chemistry of molecules
October 14	Molecules and molecular structures
October 16	Quantum chemistry and molecular spectroscopy
October 21	Approximate methods of quantum chemistry
October 23	Wrap up and review material for EXAM II
October 28	Symmetry and group theory
October 30	EXAM II
November 4	Symmetry and group theory
November 6	Symmetry and group theory
November 11	Symmetry and group theory
November 13	Symmetry, group theory and molecular spectroscopy
November 18	Computational methods of quantum chemistry
November 20	Student presentations
November 25	THANKSGIVING HOLIDAY BREAK (NO CLASS MEETING)
November 27	THANKSGIVING HOLIDAY BREAK (NO CLASS MEETING)
December 2	Student presentations
December 4	Wrap up and review material for EXAM III
December 9 and 11	READING DAYS (A&S)
December 12	EXAM III (Starts at 5:45 PM unless room is available at 5:30 PM)

UMKC Resources & Policy Statements

Please refer to the following web page and the linked resources there on for critical information regarding course policies and resources. You are expected to abide by all the rules and regulations regarding student conduct referenced in these pages. http://cas.umkc.edu/CPR/

Academic Calendar: Students are encouraged to review important add, drop or withdraw dates: http://www.umkc.edu/registrar/acal.asp

Academic Honesty: The Board of Curators of the University of Missouri recognizes that academic honesty is essential for the intellectual life of the University. Faculty members have a special obligation to expect high standards of academic honesty in all student work. Students have a special obligation to adhere to such standards. Academic dishonesty, including cheating, plagiarism or sabotage, is adjudicated through the University of Missouri Student Conduct Code and Rules of Procedures in Student Conduct Matters.

Academic Inquiry, Course Discussion and Privacy:

Faculty allowing recording - University of Missouri System Executive Order No. 38 lays out principles regarding the sanctity of classroom discussions at the university. The policy is described fully in Section 200.015 of the Collected Rules and Regulations. In this class, students may make audio or video recordings of course activity unless specifically prohibited by the faculty member.

However, the redistribution of any audio or video recordings of statements or comments from the course to individuals who are not students in the course is prohibited without the express permission of the faculty member and of any students who are recorded, including those recordings prepared by an instructor. Students found to have violated this policy are subject to discipline in accordance with provisions of Section 200.020 of the Collected Rules and Regulations of the University of Missouri pertaining to student conduct matters.

Attendance Policy: Students are expected to attend and participate in classes. Advance notice of attendance policies of academic units and individual instructors should be given, and such notice should be in writing. Students should notify instructors of excused absences in advance, where possible. Students who have an excused absence are expected to make arrangements with instructors for alternative or make-up work. Such arrangements should be made in advance of the absence, where possible. Instructors should accommodate excused absences to the extent that an accommodation can be made that does not unreasonably interfere with the learning objectives of the course or unduly burden the instructor. Attendance policies shall be applied in a non-discriminatory manner.

Campus Safety: Inclement weather, mass notification, and emergency response guide: http://www.umkc.edu/umkcalert/

Counseling and Health Services Available at UMKC:

UMKC students may experience many challenges in their lives while attending college – stress, depression, suicidality, trauma, relationship issues, health concerns, etc. As your professor I care about your success and well-being and want to make you aware of some helpful resources on campus. The UMKC Counseling Center (www.umkc.edu/counselingcenter), located at 4825 Troost in Room 206, offers a wide range of supportive services to students. Appointments can be made by calling 816.235.1635. UMKC Student Health and Wellness (http://info.umkc.edu/studenthealth/), located at 4825 Troost in Room 115, offers a full range of health care and promotion services. Appointments can be scheduled online or by calling 816.235.6133. The Mind Body Connection (www.umkc.edu/mindbody) is located in the Atterbury Student Success Center in Room 112 and offers a variety of stress-reduction services.

Disability Support Services:

To obtain disability related accommodations and/or auxiliary aids, students with disabilities must contact the Office of Services for Students with Disabilities (OSSD) as soon as possible. To contact OSSD, call (816) 235-5696. Once verified, OSSD will notify the course instructor and outline the accommodation and/or auxiliary aids to be provided. For more information go to: http://www.umkc.edu/disability/

English Proficiency Statement:

Students who encounter difficulty in their courses because of the English proficiency of their instructors should speak directly with their instructors. If additional assistance is needed, students may contact the UMKC Help Line at 816-235-2222 for assistance.

Grade Appeal Policy:

Students are responsible for meeting the standards of academic performance established for each course in which they are enrolled. The establishment of the criteria for grades and the evaluation of student academic performance are the responsibilities of the instructor.
The University grade appeal procedure is available only for the review of allegedly capricious grading and not for review of the instructor's evaluation of the student's academic performance. Capricious grading, as that term is used here, comprises any of the following:
• The assignment of a grade to a particular student on some basis other than the performance in the course;
• The assignment of a grade to a particular student according to more exacting or demanding standards than were applied to other students in the course; (Note: Additional or different grading criteria may be applied to graduate students enrolled for graduate credit in 300- and 400-level courses.)
• The assignment of a grade by a substantial departure from the instructor's previously announced standards.

Discrimination Grievance Procedures for Students:

Discrimination Grievance Procedures for Students can be found here:
http://www.umsystem.edu/ums/rules/collected_rules/grievance/ch390/grievance_390.010

Statement of Human Rights:

The Board of Curators and UMKC are committed to the policy of equal opportunity, regardless of race, color, religion, sex, sexual orientation, national origin, age, disability and status as a Vietnam era veteran. Commitment to the policy is mentored by the Division of Diversity, Access & Equity, but it is the responsibility of the entire university community to provide equal opportunity through relevant practices, initiatives and programs.

Title IX:

Under the University of Missouri's Title IX policy, discrimination, violence and harassment based on sex, gender, and gender identity are subject to the same kinds of accountability and support applied to offenses based on other protected characteristics such as race, color, ethnic or national origin, sexual orientation, religion, age, ancestry, disability, military status, and veteran status. If you or someone you know has been harassed or assaulted, you can find the appropriate resources by visiting UMKC's Title IX Office webpage (http://info.umkc.edu/title9/) or contacting UMKC's Title IX Coordinator, Sybil Wyatt (816.235.6910 or wyattsb@umkc.edu). Additionally,

you can file a complaint using UMKC's online discrimination complaint form, which is located at http://info.umkc.edu/title9/reporting/report-online/.

While most UMKC employees are required to report any known or suspected violation of Title IX, students may seek confidential guidance from the following campus locations:

UMKC Counseling Service **Volker Campus** 5110 Oak St Ste 201, Kansas City, MO 64112 Phone – (816) 235-1635 Open – Mon thru Fri – 8 am to 5 pm	**Student Health and Wellness** Volker Campus 5110-5101, Oak St Kansas City, MO 64112 Phone - (816) 235-6133 Open – Mon thru Fri – 8 am to 5 pm

UMKC Connect:

Important information is available to undergraduate students in UMKC Connect accessed through Blackboard. Throughout the term, students may receive emails regarding course grades or academic performance. Students are expected to address information posted in a timely fashion. This information may be shared with the student's Success Network made up his or her academic advisor(s) and other campus resources so that UMKC may fully support the student's success.

College of Arts & Sciences Course Policies & Resources:

Please refer to the following web page and the linked resources for critical information regarding course policies and resources. You are expected to abide by all the rules and regulations regarding student conduct referenced in these pages. http://cas.umkc.edu/CPR/

CHEM 5533 QUANTUM CHEMISTRY FALL 2019

STUDENT INFORMATION QUESTIONNAIRE

(In order for me to make my instruction more personalized and helpful, I like to learn more about students as individuals. If you would, please fill out the information requested below, and return it to me within the first 2 weeks of the semester via email. I will retain this information on file only for this semester and will not be shared with others, but you are under no obligation to provide any or all of the data requested.)

PLEASE PRINT, AND THANKS!

NAME _____

WHERE ARE YOU FROM? _____

WHAT ARE YOUR PLANS ONCE YOU FINISH YOUR DEGREE PROGRAM?

_____

PLEASE LIST THE NAMES OF COLLEGE LEVEL *CHEMISTRY* COURSES YOU HAVE TAKEN BELOW (PLEASE ALSO INDICATE WHERE THESE WERE TAKEN):

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PLEASE LIST THE NAMES OF COLLEGE LEVEL *MATH* COURSES YOU HAVE TAKEN BELOW (PLEASE ALSO INDICATE WHERE THESE WERE TAKEN):

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PLEASE LIST THE NAMES OF COLLEGE LEVEL *PHYSICS* COURSES YOU HAVE TAKEN BELOW (PLEASE ALSO INDICATE WHERE THESE WERE TAKEN):

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(Please use the back side of this page to provide me with any other relevant information, such as your class schedule and any scheduled commitments, such as work or service.)