Physics 5393 CRN 17593 - Special Topics in X-Ray and UV-vis Spectroscopy

PSCI Rm 218

Wednesday 4:30-7:20

https://www.overleaf.com/project/64e60e19956536ee4bc95727

	OFFICE HOURS	
Mark Pederson	PSCI Rm 209A	Th 2:30-4:00PM or by Appt.
Tunna Baruah		By Appt.
Eunja Kim		By Appt.

This course prepares students for understanding how core-level and valence-level spectroscopy can be used to characterize molecular and solid-state systems and to determine material composition through comparisons of calculated and measured spectra. It will provide a qualitative understanding on how electronic-, spin-, spin-orbit, vibrational- and isotopic- degrees of freedom effect measurements of spectra. The course is primarily computational. Students will learn how to use Linux-based computing paradigms on platforms that range from laptops to massively parallel computing architectures and will provide reports using LaTeX-based scientific word processing protocols. The classroom is taught using protocols that are used on a day-to-day basis for geographically separated scientists who have multi-institutional collaborations. Students will be given the opportunity to lead one 15-minute discussion during the semester and to present their class project at the end of the semester. They will have the opportunity to present their projects to experts in x-ray science at PNNL. To help students determine their class project, we will intersperse concise ideas in weekly assignments. Additional information about classroom policies may be found at: Extended Syllabus and Course Policies.

Frequently Asked Questions

Frequently asked questions may be found generally at: Frequently Asked Questions. Questions about Classroom procedures may be found at: Class processes. Questions about OVERLEAF may be found at: Overleaf Questions. Questions about NRLMOL may be found at: NRLMOL and FLOSIC Questions. Questions about Quantum Espresso may be found at: Quantum Espresso Questions. A Linux tutorial may be found at: Basic Linux Commands and questions about Linux may be found at Linux Questions. Questions about running codes on JAKAR may be found at: Jakar Questions. If you don't see the question and answer that you are looking for, please post it at: Bulletin Board For New Questions

Weekly Homework, Assignments, Reading, and Excercises

Each week, the active assignment, due on the following week, can be found at: Active Assignment - Due by 6-September 2023.

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Basic Linux Commands

The software will be used on the UTEP supercomputer jakar.utep.edu. When you login to jakar you will get an unix shell. You will have to type in the commands at the prompt which is usually a dollar sign. The following unix/linux commands are the mostly used commands.

ls	The most frequently used command in Linux to list directories
pwd	Print working directory command in Linux
cd	Linux command to navigate through directories
mkdir	Command used to create directories in Linux
mv	Move or rename files in Linux
cp	Similar usage as mv but for copying files in Linux
rm	Delete files or directories
touch	Create blank/empty files
cat	Display file contents on the terminal
clear	Clear the terminal display
less	Linux command to display paged outputs in the terminal
man	Access manual pages for all Linux commands
uname	Linux command to get basic information about the OS
whoami	Get the active username
tar	Command to extract and compress files in Linux
grep	Search for a string within an output
head	Return the specified number of lines from the top
tail	Return the specified number of lines from the bottom
diff	Find the difference between two files
zip	Zip files in Linux
unzip	Unzip files in Linux
ssh	Secure Shell command in Linux
ps	Display active processes
kill and killall	Kill active processes by process ID or name
df	Display disk filesystem information
mount	Mount file systems in Linux
chmod	Command to change file permissions
chown	Command for granting ownership of files or folders
passwd	Create or update passwords for existing users
cal	View a command-line calendar

When you login to jakar, first change your passwd to something you can easily remember. Use the passwd command for that.

vi editor

To run the code you will to edit input files. similarly, to read the output you will need to open and read the output files. These are text files.

A vi editor cheat sheet is available here:A

https://www.atmos.albany.edu/daes/atmclasses/atm350/vi_cheat_sheet.pdf

Date	Topics & Tasks	Instructor
08/30	Primers: OVERLEAF, Linux, LaTeX, NRLMOL, Library Resources, Submitting jobs on Jakar, Basics of x-ray spectra, The Bohr atom. Introduction to X-Rays. Assignments are in: Assignment 1.1	Baruah, Kim, Pederson
09/06	1s-core level (K-Edge) spectra. 2p-core level (L-edge) spectra. Comparison of Bohr-Formula to Measurement. Assignments are in: Assignment 2	Baruah
09/13	Chemical shift in C K-edge spectra. CH_4 vs CF_4. Fluorinated vs Hydrogenated diamond surfaces. Assignments are in: Assignment 3	MRP or TB
09/20	Special Seminars. Charge-induced changes in x-ray spectra. Excitonic vs Ionization core-level excitations. Assignments are in: Assignment 4	Kim
09/27	Changes in X-Ray spectra due to changes in spin states. Assignments are in: Assignment 5	Baruah
10/04	Dipole Selection Rules. Quadrapole Selection Rules. Assignments are in: Assignment 6	TB or MRP
10/11	Spin-Orbit Coupling. Assignments are in: Assignment 7	Pederson
10/18	NO CLASS UTEP-UNM Football	
10/25	Proposals for class projects are due. Quantum Tunneling of Magnetization in Molecular Magnetims and related spectroscopies. Assignments are in: Assignment 8	Pederson
11/01	Basis Sets. Self-Interaction Corrected Orbital energies. Assignments are in: Assignment 9	Pederson
11/08	Introduction to Quantum-Espresso. Assignments are in: Assignment 10	Kim
11/15	Structural Optimization of unit Cells. Assignments are in: Assignment 11	Kim
11/22	Thanksgiving Break	
11/29	Electronic Density of States. Assignments are in: Assignment 12	Kim
12/06	Frozen phonon calculations and IR and Raman Spectra. Assignments are in: Assignment 13	Kim
12/13	Presentation of Projects	Baruah, Kim, Pederson

	Required Seminars for MS Students	Speaker
9/8	Advanced Microscopy for Particle-to-Bulk Correlations in Special Nuclear Materials	Dr. E. Buck
9/15	Self-Interaction Corrections to Density Functional Theory: Overview and Applications	Dr. M.R. Pederson
9/22	From A to B on free energy landscapes via a synthesis of rare-event sampling and machine learning."	Dr. M. Tuckerman
9/29	Oxides for data and energy storage: Synthesis, crystal growth and scattering studies"	Dr. H. Nair
10/13	Relativistic Electronic Structure Theory: Approaching the Spectroscopic Accuracy	Dr. Xiaosong Li
10/20	Extended Lagrangian Shadow Molecular Dynamics	Dr. A. Niklasson
10/27	TBA	TBA
11/3	Informing Nuclear Forensics Research with Spectroscopy and Supercomputers	Dr. A. Shields
11/10	Quantinuuum	Dr. K. Spendier
11/17	Crystal structure predictions with graph neural networks	Dr. C. Sutton
12/1	Makeup Seminar	TBD
12/8	TBD	Raphaele Clément

Active Assignment - Due by 6-September 2023

Assignment 1.1

Person	Atom	Z	K-Edge	L_1-Edge	$E_K(Bohr)$	E_K(DFT)
Pederson Acter Adhikari Vlazquez Juarez Lopez MacDonald Muthunayakakkage Oyetunji	Phosphorus(P)	15	2143.54	189.0	3060.	

Table 1: Go to https://physics.nist.gov/PhysRefData/XrayTrans/Html/search.html, In the left-hand "By Elements" tab, find the atom that has and atomic symbol that is close to the first letter in your last name or first name. Select that atom, In the "Energy/Wavelength" tab enter a range from 0 to 1000000 eV. Then select "Get Transitions". Put the energies for the 1s-core (K-Edge) and 2p- (L_1-edge) (in eV) in your row of Table 1 by clicking on "Assignment 30 August.tex" in the left-hand window of the Overleaf Menu.Then, use the Bohr formulae to estimate the atomic charge of your atom. For the 1s-energy (K-edge), the Bohr Formula would tell that $E_K = 13.6Z^2$.

Assignment 1.2

In the course material folder download the file nrlmol-simple.tar.gz and move it to your linux-based laptop or JAKAR. Open the file using the following commands:

```
gunzip nrlmol-simple.tar.gz
tar -xf nrlmol-simple.tar
cd nrlmol-simple
./compile_it
mkdir MyFirstAtom
cd MyFirstAtom
../codes/mpnrlmol.ser
../codes/mpnrlmol.ser
```

Assignment 1.3

Familiarize yourself with linux commands and the vi editor.

```
cd mv ls chmod cp rm mkdir ps vi
```

Assignment 1.4

Read Chapter 1 and 2 (Pages 1-10) of: https://docs.xrayabsorption.org/tutorials/XAFS_Fundamentals.pdf

Useful Resources

1. Web of Science: https://www.webofscience.com/wos/woscc/basic-search
2. NRLMOL/FLOSIC Tutorials
   - https://quantum.utep.edu/new_nrlmol/nrlmoldoc_main.html
   - https://www.youtube.com/watch?v=QQE6oSBo5ts
3. X-Ray Emission Spectra: https://en.wikipedia.org/wiki/X-ray_emission_spectroscopy
4. X-Ray Absorption Spectra: https://en.wikipedia.org/wiki/X-ray_absorption_spectroscopy
5. X-Ray tutorial: https://docs.xrayabsorption.org/tutorials/XAFS_Fundamentals.pdf
6. Experimental x-ray lines, ordered by atom, may be found at:results can be found at: https://physics.nist.gov/PhysRefData/XrayTrans/Html/search.html
7. Experimental x-ray lines, ordered by energy, may be found at:results can be found at: http://xdb.lbl.gov/Section1/Table_1-3.pdf
8. To find the Linux tutorial click here: Basic Linux Commands.

1 Semester Reading - Available Online

- The role of dipole selection rules: **New Theoretical Model for the Diamond 1s-core exciton** K.A. Jackson and M.R. Pederson, Phys. Rev. Lett. **67**, 2521 (1991) https://doi.org/10.1103/PhysRevLett.67.2521. Relevance to Assignment 3 and Assignment 8
- The role of spin-orbit in x-ray spectral shapes: **Electronic structure of the molecule-based magnet $Mn(N(CN)_2)_2$ from theory and experiment**, M. R. Pederson, A. Y. Liu, Tunna Baruah, E. Z. Kurmaev, A. Moewes, S. Chiuzbaian, M. Neumann, C. R. Kmety, K. L. Stevenson, and D. Ederer, Phys. Rev. B. **66**, 014446 (2002). https://doi.org/10.1103/PhysRevB.66.014446. Relevance to Assignment 5 and Assignment 7 and .
- Determining coordination from x-ray spectra **Characterization of pentavalent and hexavalent americium complexes in nitric acid using X-ray absorption fine structure spectroscopy and first-principles modeling**, Catherine Riddle, Kenneth Czerwinski, Eunja Kim, Patricia Paviet, Philippe Weck, Frederic Poineau & Steven Conradson, Journal of Radioanalytical and Nuclear Chemistry, **309** (2016), https://link.springer.com/article/10.1007/s10967-016-4704-x.
- Challenges for calculating optically silent charge-transfer states: **Density functional study on a light-harvesting carotenoid-porphyrin-C60 molecular triad**, T. Baruah and M.R. Pederson, J. Chem. Phys. 125, 164706 (2006); https://aip.scitation.org/doi/10.1063/1.2360265. Relevant to Assignment 4
- The role of self-interaction corrections: **Chapter Eight - Self-Interaction Corrections Within the Fermi-Orbital-Based Formalism** Mark R Pederson and Tunna Baruah, Advances in Atomic Molecular and Optical Physics **64** 153-180 (2015); https://doi.org/10.1016/bs.aamop.2015.06.005.
- Characterization of Transition Metal Complexes with x-rays **Simulating Valence-to-Core X-ray Emission Spectroscopy of Transition Metal Complexes with Time-Dependent Density Functional Theory**, Y. Zhang, S. Mukamel, M. Khalil, N. Govind, J. Chem. Theory Comput, 11, 5804 (2015).
- FIX TITLE AND REFERENCE. Sharmin Akter,Jose. Vargas,Kamal Sharkas,Juan E. Peralta, Koblar A. Jackson, and Tunna Baruah, https://doi.org/10.1021/acs.jctc.5b00763.

- Basis Set Effects for Dipole-Coupled Systems **How well do self-interaction corrections repair the overestimation of static polarizabilities in density functional calculations?**, Sharmin Akter,Jose. Vargas,Kamal Sharkas,Juan E. Peralta, Koblar A. Jackson, and Tunna Baruah, : Phys. Chem. Chem. Phys.**23**, 18678 (2021). DOI:10.1039/d0cp06512a.

- Vibrational splittings in X-Ray Spectra (?) Infrared intensities and Raman-scattering activities within density-functional theory, Dirk Porezag and Mark R. Pederson Phys. Rev. B **54** 7830 (1996). https://doi.org/10.1103/PhysRevB.54.7830.

- Uncertainties, or lack thereof?, in core-level shifts due to basis sets: **Optimization of Gaussian basis sets for density-functional calculations**, Dirk Porezag and Mark R. Pederson, Phys. Rev. A **60**, 2840 (1999) https://doi.org/10.1103/PhysRevA.60.2840.

Assignment 2

Assignment

Comparison of 1s-DFT eigenvalue to Experimental Calculation

Using your version of NRLMOL, we will first compare the lowest density functional eigenvalue to the measured x-ray spectra. The example below is set up for Zinc (Z=30). To perform a calculation on the problem assigned to you create a file called "CLUSTER" with the correct value of Z. See Table 2 for your assigned atom. Also, put your results in this table which can be found in the overleaf directory nameed "Assignment 6 September" in the OVerleaf Assignments directory. Then run the code in this directory.

```
GGA-PBE*GGA-PBE          (DF TYPE EXCHANGE*CORRELATION)
TD                       (TD, OH, IH, X, Y, XY, ... OR GRP)
1                        (NUMBER OF INEQUIV. ATOMS IN XENON)
0.00 0.00 0.00  30 ALL  (R, Z, PSEUDOPOT. TYPE FOR XENON)
0.0 0.0                  (NET CHARGE AND NET SPIN)rr
```

RESULT (FROM FILE CALLED EVALUES):

```
 SUMMARY OF EVALUES AND THEIR OCCUPANCIES:
    1  REP:  1  DEG:  1  ENERGY:   -345.633      OCC:    1.00000  <=1S Core Eigenvalue
    2  REP:  1  DEG:  1  ENERGY:   -41.5991      OCC:    1.00000
    3  REP:  2  DEG:  3  ENERGY:   -36.6622      OCC:    1.00000
    4  REP:  1  DEG:  1  ENERGY:   -4.59469      OCC:    1.00000
    5  REP:  2  DEG:  3  ENERGY:   -3.02714      OCC:    1.00000
    6  REP:  2  DEG:  3  ENERGY:  -0.388052      OCC:    1.00000
    7  REP:  3  DEG:  2  ENERGY:  -0.388052      OCC:    1.00000
    8  REP:  1  DEG:  1  ENERGY:  -0.213817      OCC:    1.00000 <= Highest Eigenvalue
    9  REP:  2  DEG:  3  ENERGY:  -0.387849E-01  OCC:    0.00000
   10  REP:  1  DEG:  1  ENERGY:   0.706944E-01  OCC:    0.00000
```

The above energies are in Hartree atomic units. To convert to electron volts, they need to be multiplied by 27.2116. Therefore for Zn, an estimate of the K-Shell ionization energy is 9405.2 eV. The estimate from the Bohr Hydrogen approximately is $3.6x(30)^2 = 12240eV$.

1.1 Delta SCF calculations for core-level Excitations

Study the files that are in the nrlmol-simple directory and the espcially the directories called K-Shell and L-Shell. By running those codes, try to understand what is needed to calculate X-ray ionizations.

Possible 5393 Project:Automating extraction of core-level excitations in molecules containing identical atoms in chemically different environments.

2 Assignment 3

Status: This assignment is under construction. Everyone is encouraged to perform assignments prior to class discussion and prior to the Assignment date. If so, please check back on the actual date of the assignment as there will be questions and extensions to the assignments based upon student feedback during the classroom.

This weeks assignment aims to learn how to optimize molecular geometries and to analyze how the K-edge is expected to change when an atom (in this case a Carbon atom) neighbors hydrogens as compared to

fluorine atoms. Sometimes these shifts are referred to as chemical shifts and sometimes they are referred to as charge-transfer shifts.

Please download "Assignment3.tar.gz" from the course material folder on Overleaf.

Possible 5393 Project:Revisiting core-level shifts in hydrogenated and fluorinated diamond surfaces

Assignment 4

Status: This assignment is under construction. Everyone is encouraged to perform assignments prior to class discussion and prior to the Assignment date. If so, please check back on the actual date of the assignment as there will be questions and extensions to the assignments based upon student feedback during the classroom.

Assignment 4.1

Read: The role of dipole selection rules: **New Theoretical Model for the Diamond 1s-core exciton** K.A. Jackson and M.R. Pederson, Phys. Rev. Lett. **67**, 2521 (1991) https://doi.org/10.1103/PhysRevLett.67.2521.

Assignment 4.2

Assignment20Sept.tar.gz. Look at the example exciton and x-ray calculations for the Zn Atom. Calculate the 1s-core level binding energy and the lowest exciton level for one of the examples and place your answers in Table 3.

Assignment 4.3

Calculate the Ionization energy of Li. Calculation the electron Affinity of F. Then Try to reproduced the calculated energy difference by performing a calculation on a LiF molecule with the Li and F separated by 100 atomic units.

Volunteer Needed: I need one volunteer to lead a 15-minute discussion on the results next week. Please put your name here if you volunteer:

Possible 5393 Project:Transition energies from core levels in solution to neighboring water molecules or to onsite-excitons require special techniques.

Assignment 5

Status: This assignment is under construction. Everyone is encouraged to perform assignments prior to class discussion and prior to the Assignment date. If so, please check back on the actual date of the assignment as there will be questions and extensions to the assignments based upon student feedback during the classroom.

Please read: The role of dipole selection rules: **New Theoretical Model for the Diamond 1s-core exciton** K.A. Jackson and M.R. Pederson, Phys. Rev. Lett. **67**, 2521 (1991) https://doi.org/10.1103/PhysRevLett.67.2521.

Assignment 5.1

Volunteer Needed: I need a volunteer to discuss the difference between excitation energies and allowable excitation transtions.

Please complete table: 3.

Possible 5393 Project:Creating software for X-ray absorption spectra within more exact exchange-correlation methods would be difficult but worthwhile.

Assignment

Possible 5393 Project:Calculations of core-level exciton binding energies relative to core-level ionization.

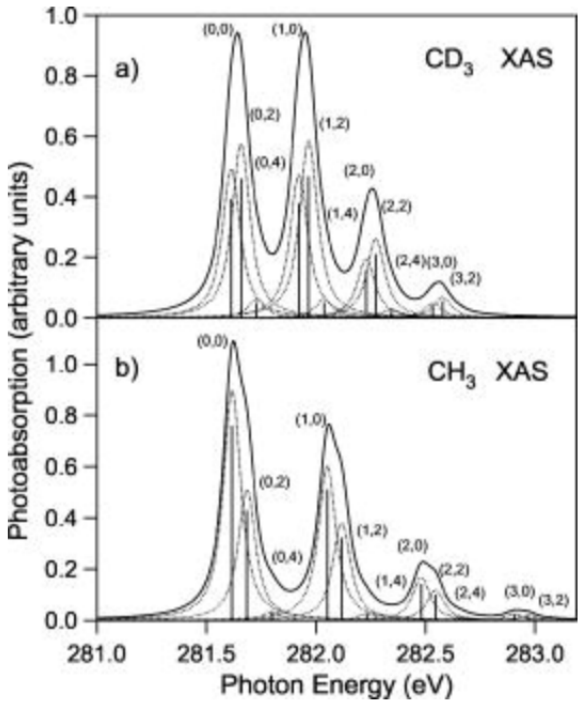

Figure 1: In this figure (by E the 1s-core level spectra is shown. By performing calculations with the CLUSTER file here, can you determine the splitting of the 1s-core levels due to spin polarization?

Assignment 6

Status: This assignment is under construction. Everyone is encouraged to perform assignments prior to class discussion and prior to the Assignment date. If so, please check back on the actual date of the assignment as there will be questions and extensions to the assignments based upon student feedback during the classroom.

In Fig. 1 the measured core-level splitting of the 1s-core levels due to spin polarization and vibration is shown (Full text of the paper can be found here: https://doi.org/10.1063/1.2822246). Please add your calculations to Table 4.

Assignment 6.1

```
GGA-PW91*GGA-PW91          (DF TYPE EXCHANGE*CORRELATION)
C3V                        (TD, OH, IH, X, Y, XY, ... OR GRP)
2                          (NUMBER OF INEQUIV. ATOMS IN MOLECULE)
     -0.00000800            -0.00000800            -0.00000800   6   ALL
      0.83670000             0.83670000            -1.67346400   1   ALL
0.0 1.0                    (NET CHARGE AND NET SPIN)
```

Assignment 6.2

In Table 4, each student has been asked to calculate the 1s-core level splitting for the methyl radical at its equilibrium geometry and at one additional geometry. Please also perform the calculation at the second geometry assigned to you. https://doi.org/10.1063/1.2822246

Possible 2-3 person 5393 Project:Since experimental characterization, via x-rays, often deals with differences of energies, are basis sets, level of theory, level of self-consistency, imporTant? Which of these is the accuracy limiting feature?

Assignment 7

Status: This assignment is under construction. Everyone is encouraged to perform assignments prior to class discussion and prior to the Assignment date. If so, please check back on the actual date of the assignment as there will be questions and extensions to the assignments based upon student feedback during the classroom.

Read about origins of spin-orbit coupling from a perspective of classical electricity and magnetism. Read through the discussion on the Thomas Precession.
https://en.wikipedia.org/wiki/Spinorbit_interaction

Read: The role of spin-orbit in x-ray spectral shapes: **Electronic structure of the molecule-based magnet** $Mn[N(CN)_2]_2$ **from theory and experiment** , M. R. Pederson, A. Y. Liu, Tunna Baruah, E. Z. Kurmaev, A. Moewes, S. Chiuzbăian, M. Neumann, C. R. Kmety, K. L. Stevenson, and D. Ederer, Phys. Rev. B. **66**, 014446 (2002). https://doi.org/10.1103/PhysRevB.66.014446. Relevance to Assignment 5 and Assignment 7

Assignment 8

Status: This assignment is under construction. Everyone is encouraged to perform assignments prior to class discussion and prior to the Assignment date. If so, please check back on the actual date of the assignment as there will be questions and extensions to the assignments based upon student feedback during the classroom.

Assignment 9

Status: This assignment is under construction. Everyone is encouraged to perform assignments prior to class discussion and prior to the Assignment date. If so, please check back on the actual date of the assignment as there will be questions and extensions to the assignments based upon student feedback during the classroom.

Assignment 10

Status: This assignment is under construction. Everyone is encouraged to perform assignments prior to class discussion and prior to the Assignment date. If so, please check back on the actual date of the assignment as there will be questions and extensions to the assignments based upon student feedback during the classroom.

Assignment 11

Status: This assignment is under construction. Everyone is encouraged to perform assignments prior to class discussion and prior to the Assignment date. If so, please check back on the actual date of the assignment as there will be questions and extensions to the assignments based upon student feedback during the classroom.

Assignment 13

Status: This assignment is under construction. Everyone is encouraged to perform assignments prior to class discussion and prior to the Assignment date. If so, please check back on the actual date of the assignment as there will be questions and extensions to the assignments based upon student feedback during the classroom.

Assignment 12

Status: This assignment is under construction. Everyone is encouraged to perform assignments prior to class discussion and prior to the Assignment date. If so, please check back on the actual date of the assignment as there will be questions and extensions to the assignments based upon student feedback during the classroom.

Compare vibrational modes of CH4, as calculated with NRLMOL and specsym, to those of Quantum Espresso, Determine the isotope shift when one of the hydrogen atoms turns into a deuterium or tritium. Determine the isotope shift when the carbon atoms becomes a ^{13}C. For this project you may download Assignment13.tar.gz from the Course Material Folder.

Frequently Asked Questions

Class processes

- Where can I access full information about he syllabus Try this link: Extended Syllabus and Course Policies.

Overleaf Questions

- How do I understand the formats of the Tables that we need to complet for the course?
- Why is it so difficult to control the placement of tables in LaTeX? Good Question. If anyone could make understanding all the intracies of Overleaf/LaTeX tables, it would be great to have them volunteer to give such a tutorial in plain language.

Linux Questions

- Who founded Linux named after? Patrick Vokerding. See: `https://en.wikipedia.org/wiki/Patrick_Volkerding`.

NRLMOL and FLOSIC Questions

- Where can I download the classroom optimized version of the code From this overleaf file in the Course Material Folder.

Quantum Espresso Questions

- Where does the class meet? Rm 218 Physical Sciences Building.

Jakar Questions

- How do I get an account on jakar? We have arranged it for you. Please check your UTEP email.

Bulletin Board For New Questions

Person	Atom	Z	K-Edge	L_1-Edge	$E_K(Bohr)$	E_K(DFT)	ΔSCF
Pederson	Xe	30	9661.	1196.7	12240.	9405.2	9568.224
Acter	Be						
Adhikari	Ne						
Vlazquez	Mg						
Juarez	Ar						
Lopez	Ca						
MacDonald	Zn						
Muthunayakakkage	Kr						
Oyetunji	Rb						

Table 2: Go to https://physics.nist.gov/PhysRefData/XrayTrans/Html/search.html, In the left-hand "By Elements" tab, find the atom that has been assigned to you. Select that atom, In the "Energy/Wavelength" tab enter a range from 0 to 1000000 eV. Then select "Get Transitions". Put the energy (in eV) in your row of the above talbe by clicking on "Assignment 6 September.tex" in the left-hand window of the Overleaf Menu (in the assingments folder). Then, use the Bohr formulae to estimate the atomic charge of your atom. For the 1s-energy (K-edge), the Bohr Formula would tell that $E_K = 13.6Z^2$.

Person	Atom	Z	K-Edge	S-S Exciton	S-P Exciton	$\Delta\lambda$(DFT)	ΔSCF
Pederson	Zn	30			12240.		
	Be						
	Ne						
	Mg						
	Ar						
	Ca						
	Zn						
	Kr						
	Rb						

Table 3: Go to https://physics.nist.gov/PhysRefData/XrayTrans/Html/search.html.

Person	R_o	Δ_{1s}^{spin}(eV)	R_o	$\Delta_{1s}^{spin}(R)$ (eV)
Oyetunji	(0.8367,0.8367,-1.6734)		(1.0,1.0,2.0)	
Juarez	(0.8367,0.8367,-1.6734)		(0.95,0.95,-1.90)	
Lopez	(0.8367,0.8367,-1.6734)		(0.92,0.92,-1.84)	
Pederson	(0.8367,0.8367,-1.6734)		(0.90,0.90,1.80)	
Juarez	(0.8367,0.8367,-1.6734)		(0.88,0.88,-1.76)	
Acter	(0.8367,0.8367,-1.6734)		(0.85,0.85,-1.70)	
Adhikari	(0.8367,0.8367,-1.6734)		(0.80,0.80,-1.60)	
Vlazquez	(0.8367,0.8367,-1.6734)		(0.75,0.75,-1.50)	
MacDonald	(0.8367,0.8367,-1.6734)		(0.72,0.72,-1.44)	
Muthunayakakkage	(0.8367,0.8367,-1.6734)		(0.97,0.97,-1.94)	

Table 4: Starting with the CLUSTER file in Section Assignment 6 determine the core-level splitting for the 1s manifold. Compare it to Fig. 1. Put your calculated results in the empty columns of this table.

Extended Syllabus and Course Policies

Addenda to Syllabus
The University of Texas at El Paso
Physics Department
Syllabus for Physics 5393

COURSE INFORMATION
Physics 5393: Computational X-Ray Spectra
CRN: 12345
Term: Fall 2023
Delivery Method: In-person
Meeting Day and Time: Wednesdays, 4:30 pm – 7:20 pm
Location: PSI-218

INSTRUCTOR INFORMATION
Mark R Pederson[a], Professor
Tunna Baruah[b], Professor
Eunja Kim[c], Professor
Written Communication should be email
[a]Office Location: PSCI, Rm 209; Office Hours: Wed 4:00-4:30, M 4:00-5:00

COURSE DESCRIPTION This course prepares students for understanding how core-level and valence-level spectroscopy can be used to characterize molecular and solid-state systems and to determine material composition through comparisons of calculated and measured spectra. This course is driven by the need to prepare students for careers in DOE labs that are tasked with continual improvements of x-ray spectroscopy. It will provide a qualitative understanding on how electronic-, spin-, spin-orbit, vibrational- and isotopic- degrees of freedom effect measurements of spectra. The course is primarily computational. Students will learn how to use linux-based computing paradigms on platforms that range from laptops to massively parallel computing architectures and will provide reports using LaTeX-based scientific word processing protocols.

COURSE OBJECTIVES AND UNIVERSITY LEARNING OUTCOMES: By the end of this course students will be prepared for calculating basic problems in several spectroscopies that are related to x-ray absorption.

- Fluency in Linux-Based Commands for Computing
- Ability to summarize scientifically formatted resports through Overleaf and LaTeX.
- Expertise in determining equilibrium geometries of simple molecular systems.
- Expertise in calculating core- and valence- level ionization energies of atoms, molecules and molecular systems.
- Familiarity with chemical-, electrical-, isotopic-, spin-orbit-, and vibrational- signatures in x-ray spectra.
- Understanding of simple relativistic effects on core-level spectroscopies.

Required Materials and Resources:
WORK IN PROGRESS
ASSIGNMENTS AND GRADING:
Students are expected to hand in their assignments at the beginning of the Wednesday class each week.
TECHNOLOGY REQUIREMENTS: Students must have a lap top and must learn how to use linux so they can perform assigned calculations.
ATTENDENCE AND PARTICIPATION:

- We will follow standard UTEP guidelines for health issues. Students with illnesses may be excused from class but may be asked to provide a note from the doctor.
- MS Science Students must attend all seminars and Wednesday Evening classes.
- In lieu of attending Friday Physics Seminars, Students that are not majoring in physics may prepare three fifteen minute high-school level introductory classes on x-ray spectroscopy. They will be asked to present one of these presentations as part of their final exam.

EXCUSED ABSENCES AND COURSE DROP POLICY
According to UTEP Catalog, "At the discretion of the instructor, a student can be dropped from a course because of excessive absences or lack of effort. A grade of "W" will be assigned before the course drop deadline and a grade of "F" after the course drop deadline." See Policies and Regulations in the UTEP Undergraduate Catalog for a list of excuse absences. You will not be dropped from the course. However, if you feel that you are unable to complete the course successfully, please let me know and then contact the Registrar's Office to initiate the drop process. If you do not, you are at risk of receiving an "F" for the course.
MAKE-UP WORK
Make-up work will be given only in the case of a documented emergency. Note that make-up work may be in a different format than the original work, may require more intensive preparation, and may be graded with penalty points. If you miss an assignment or class and the reason is not considered excusable, you will receive a zero. It is therefore important to reach out lecturers in advance if at all possible—and explain with proper documentation if you missed a given course requirement. Once a deadline has been established for make-up work, no further extensions or exceptions will be granted. Make up work will entail any of the following items:

ALTERNATIVE MEANS OF SUBMITTING WORK IN CASE OF TECHNICAL ISSUES
I strongly suggest that you submit your work with plenty of time to spare in the event that you have a technical issue with the course website, network, and/or your computer. I also suggest you save all your work (answers to discussion points, quizzes, exams, and essays) in a separate Word document as a backup. This way, you will have evidence that you completed the work and will not lose credit. If you are experiencing difficulties submitting your work through Blackboard, please contact the UTEP Help Desk. You can email me your backup document as a last resort. INCOMPLETE GRADE POLICY Incomplete grades may be requested only in exceptional circumstances after you have completed at least half of the course requirements. Talk to me immediately if you believe an incomplete is warranted. If granted, we will establish a contract of work to be completed with