Lectures (MON & THU):

Morning 8–9 AM, LH 316 — Groups 3, 5, 7, 11, 12

Afternoon 15:30–16:30, LH 108 — Groups 1, 2, 4, 6, 8, 9, 10

CML1001

Structural Insights into Atoms & Molecules

Introduction to Quantum Chemistry and Spectroscopy

Department of Chemistry . Indian Institute of Technology Delhi

Semester I . 2026-27 . Welcome to Class 1

3 Credits | L-T-P 2-1-0 | Relative grading | Course material: Moodle

01 Meet the Team

HK

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! **Email etiquette:** Write only from your institute email ID. Put **"CML1001"** in the subject, and include your **name, entry number and group ID.**

Contact your own group TA (tutor) for all tutorial questions and doubts.

02

What You'll Explore

BEFORE MID-SEM

- Origin of quantum mechanics; postulates of QM
- Schrodinger equation & model systems: particle in a box (electronic transitions, free-electron models)
- Electronic spectroscopy
- Rigid rotor & rotational transitions; rotational spectroscopy

AFTER MID-SEM BREAK

- Hydrogen atom & hydrogenic orbitals
- Chemical bond of simplest molecules (H2+, H2); bonding & anti-bonding molecular orbitals
- Harmonic oscillator & vibrational transitions in diatomics; vibrational spectroscopy
- Variational theorem & LCAO-MO

03 Course Modules

#	Topic	Hrs	CLO
1	Schrodinger equation & model systems: particle in a box (electronic transitions, free-electron models)	**4**	CLO 1
2	Harmonic oscillator & vibrational transitions	**4**	CLO 1
3	Rigid rotor & rotational transitions	**3**	CLO 1
4	Hydrogen atom & hydrogenic orbitals	**3**	CLO 1
5	The chemical bond of simplest molecules: H2+ and H2	**3**	CLO 1
6	Concept of bonding & anti-bonding molecular orbitals	**2**	CLO 1
7	Variational theorem & LCAO-MO	**4**	CLO 1
8	Electronic spectroscopy for structure determination	**5**	CLO 1

Total: 28 contact hours . All modules map to CLO 1

04

Tutorial Sheets

A new tutorial sheet is released topic-wise. Solve it before your session, then work the problems with your TA.

Sheet	Topics
0	Mathematics primer
1	Origin of QM; postulates & QM formalism (wavefunction, operators, uncertainty)
2	Schrodinger equation & model systems (free particle, particle-in-a-box); rigid rotor & rotational transitions
3	Hydrogen atom & hydrogenic orbitals; H2+ and H2
4	Harmonic oscillator & vibrational transitions
5	Bonding / anti-bonding MOs; variational theorem & LCAO-MO

Sheet 0 is a maths primer. A short quiz is given on alternate tutorials (Tutorial Quizzes = 10%). Bring your doubts - your TA will help you work through them.

05

Tutorial Schedule

Which sheet is discussed each week, and when a Tutorial Quiz is held. Dates cover the three tutorial slots - check your group's day on the group slide.

Tutorial	Dates (Tue / Wed / Thu / Fri)	Sheet	Tutorial Quiz
Tutorial 1	28 Jul / 29 Jul / — / 31 Jul	**Sheet 1**	—
Tutorial 2	4 Aug / 5 Aug / — / 7 Aug	**Sheet 1**	**Quiz**
Tutorial 3	11 Aug / 12 Aug / — / 14 Aug	**Sheet 1**	—
Tutorial 4	18 Aug / 19 Aug / — / 21 Aug	**Sheet 2**	**Quiz**
Tutorial 5	25 Aug / 2 Sep / — / 28 Aug	**Sheet 2**	—
Tutorial 6	1 Sep / 9 Sep / 3 Sep / —	**Sheet 2**	**Quiz**
Tutorial 7	8 Sep / 23 Sep / — / 11 Sep	**Sheet 3**	—
Tutorial 8	22 Sep / 7 Oct / — / 25 Sep	**Sheet 3**	**Quiz**
Tutorial 9	6 Oct / 10 Oct / — / 9 Oct	**Sheet 3**	—
Tutorial 10	13 Oct / 14 Oct / — / 16 Oct	**Sheet 4**	**Quiz**
Tutorial 11	27 Oct / 21 Oct / — / 23 Oct	**Sheet 4**	—
Tutorial 12	3 Nov / 28 Oct / — / 30 Oct	**Sheet 5**	**Quiz**
Tutorial 13	10 Nov / 4 Nov / — / 6 Nov	**Sheet 5**	—

Semester Timeline - Mark These Dates

Semester I 2026-27 . Classes begin Mon 27 Jul . Tutorials begin week of 28 Jul

COMMON QUIZ 1	MID-TERM EXAM	COMMON QUIZ 2	MAJOR / FINAL	TUTORIAL QUIZ
Tue 1 Sep	12-17 Sep	Tue 27 Oct	19-25 Nov	alternate tutorials
10% of grade	30% of grade	10% of grade	40% of grade	10% of grade

When you're evaluated

Quiz 1 1 Sep **Mid-Term** 12-17 Sep
Quiz 2 27 Oct **Major** 19-25 Nov
Tutorial quizzes on alternate tutorials (~every 2 weeks)

Tutorial sheets

Released topic-wise as **Sheets 0-5** (Sheet 0 = maths primer), from week of 28 Jul. Solve each before your session.

Holidays / breaks: 15 Aug . 26 Aug . 4 Sep . Sem break 27 Sep-4 Oct . 20 Oct . 8-9 Nov . 24 Nov . Last teaching day 17 Nov

06

How Tutorial (TA) Sessions Work

1

Purpose - clear your doubts

Tutorials clear conceptual doubts in the course that can't be handled individually during lectures. Bring your questions.

2

Solve practice problems

You'll work through practice problems from the tutorial sheet with your TA and peers - the best way to prepare for exams.

3

Evaluated by a short quiz

Your TA gives a short quiz to assess you. These Tutorial Quizzes count for 10% of the course grade.

4

Be on time - attendance

Attendance & the quiz begin within 5 minutes of the start. Only your group TA handles tutorial attendance and marks.

Come prepared: attempt the tutorial sheet beforehand and bring the doubts you couldn't resolve in class - your TA will help you work through them.

07

Your Tutorial Group & TA

Find your group below - note your TA, hall and time. Contact your group TA for all tutorial doubts, attendance & marks.

Grp	Entry No.	Tutorial TA	Size	Tutorial (day · time · hall)
1	2022CYZ8611	**Navneet**	32	LH 604 · Wed 11:00 AM–12:00 PM
2	2022CYZ8613	**Anmol**	32	LH 519 · Wed 11:00 AM–12:00 PM
3	2024CYZ8152	**Saumya**	32	LH 521 · Wed 11:00 AM–12:00 PM
4	2024CYZ8638	**Maria Amin**	32	LH 413.2 · Wed 11:00 AM–12:00 PM
5	2023CYZ8640	**Jagriti**	32	LH 519 · Wed 2:00–3:00 PM
6	2024CYZ8154	**Mathivathani JR**	31	LH 313.2 · Wed 11:00 AM–12:00 PM
7	2024CYZ8124	**Jyoti Bharti**	32	LH 313.4 · Wed 11:00 AM–12:00 PM
8	2024CYZ8156	**Malisetty Ravi Teja**	31	LH 517 · Wed 11:00 AM–12:00 PM
9	2024CYZ8164	**Zainab Fatima**	31	LH 413.4 · Wed 11:00 AM–12:00 PM
10	2024CYZ8133	**Deepak Kumar Pradhan**	32	LH 521 · Tue 11:00 AM–12:00 PM
11	2024CYZ8138	**Nitish Rani**	30	LH 521 · Wed 1:00–2:00 PM
12	2024CYZ8162	**Biswajit Samal**	30	LH 521 · Fri 1:00–2:00 PM

Contact only your own group TA (tutor) for tutorial doubts, attendance and marks.

08

How You're Graded

10%

Quiz 1 . 1 Sep

10%

Quiz 2 . 27 Oct

10%

Tutorial Quizzes

30%

Mid-Term Exam . 12-17 Sep

40%

Major / Final Exam . 19-25 Nov

Relative grading. *No re-quiz for any quiz (common or tutorial). Re-Minor & Re-Major per institute rules.*

09

Attendance Policy

As per institute norms

75%

Minimum attendance required

Below 75% -> one grade lower than earned (e.g. an A becomes A(-))

Attendance & discussions on Acadly

- Install the Acadly app on your phone.
- It's Bluetooth enabled - keep it turned ON during class.
- When the instructor starts attendance, mark yourself present.
- Use Acadly for in-class discussions - you can even post anonymously.

1. **Attend all lectures & tutorials.** Follow institute attendance rules / norms.
2. **Medical exceptions** Only with a medical certificate from IITD Hospital.
3. **No late certificates** None considered once the exam is over.
4. **Enter on time** Attendance/quiz begins within 5 min of the start.

10 Ground Rules & Integrity

General conduct

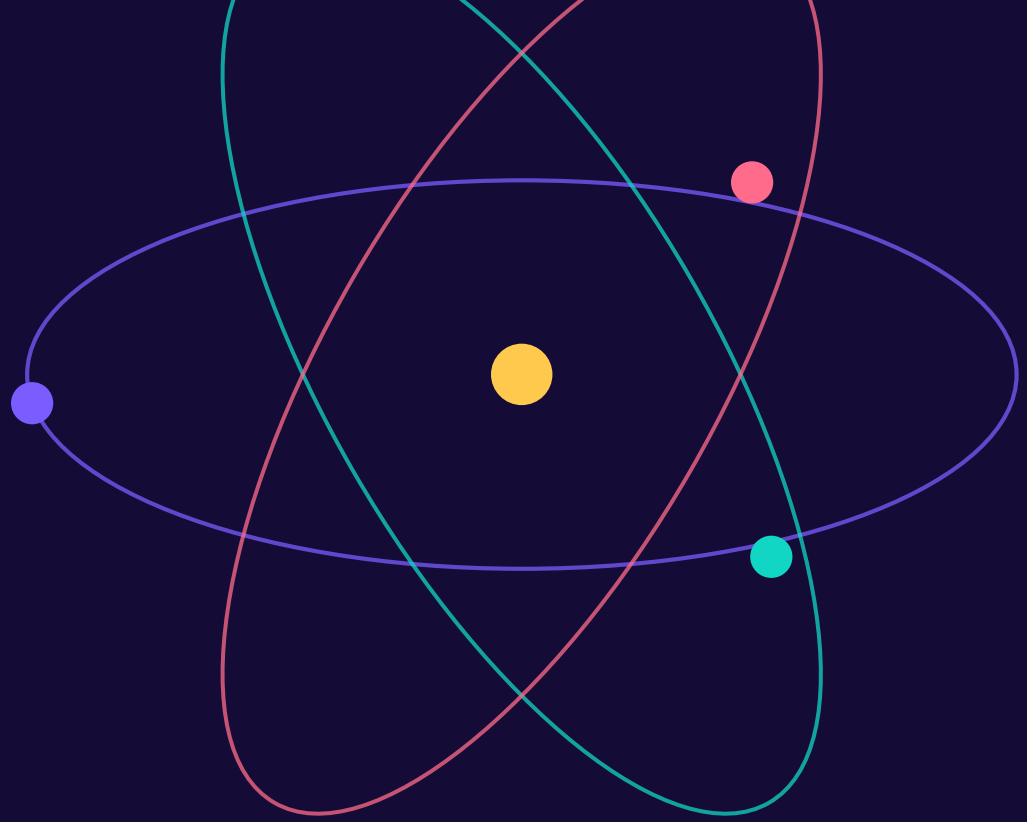
- Enter lecture/tutorial classes on time.
- Always email from your institute ID (name, entry no. & group ID in the subject).
- Contact your group TA for tutorial questions/doubts - only your tutor handles tutorial attendance & marks.
- For any other course help, contact the instructors / coordinator.

Exams & integrity

- Clear doubts on graded papers within the given time frame - afterwards marks are frozen.
- No unfair means (cheating, proxy attendance). Violations -> disciplinary action & "F" in the course.
- No re-quiz for any quiz (common + tutorial). Re-Minor & Re-Major per institute rules.

11 Reference Textbooks

1. **Elements of Physical Chemistry** P. Atkins & J. de Paula - 7th Ed, 2017
2. **Quantum Chemistry** D. A. McQuarrie - 2nd Ed, University Science Books, 2008
3. **Physical Chemistry: A Molecular Approach** D. A. McQuarrie & J. D. Simon - Viva Books, 1st South Asian Ed
4. **Physical Chemistry** Ira N. Levine - McGraw Hill, 11th Ed, 2019
5. **Quantum Chemistry** Ira N. Levine - PHI Learning, 6th Ed, 2009



Stay curious, keep questioning,

and enjoy exploring the quantum world!