

CHM 621A

Chemical Binding

First course handout

Mainak Sadhukhan

Indian Institute of Technology Kanpur

- Recapitulation of quantum mechanics
- One electron systems : Hydrogenic atoms and Dihydrogen cation
- Many-electron atoms : Approximate methods
- Valence Bond and Molecular orbital Theory: Hückel MO theory
- Hartree-Fock Theory of many-electron systems
- Electron correlation
- Free-electron gas and glimpses of electron structure in solid state
- Basics of some beyond-Hartree-Fock theories
- Glimpses of electron density-based methods
- Bond vibrations and normal modes

- Assignments will be given for practice
- Three quizzes will be arranged. Each quiz will cover 20% marks.
- In video question will cover 20% marks.
- No mid-sem examination will be arranged
- End-semester examination will cover 20% marks
- No pro-rating is admissible
- End-sem make-up can only be admissible for medical emergency, properly approved by authorities (SPGC/SUGC)

Books

- ① I.N. Levine, Quantum Chemistry, Fifth edition, Pearson Education (2000).
- ② P. W. Atkins and R. S. Friedman, Molecular Quantum Mechanics, Third edition, Oxford University Press (1997).
- ③ L. Pauling and E. B. Wilson, Introduction to Quantum Mechanics: With Applications to Chemistry, Dover (1985)
- ④ A. Szabo and N. S. Ostlund, Modern Quantum Chemistry, Dover (1996).
- ⑤ R. Parr and W. Yang, Density functional theory of atoms and molecules, Oxford University Press (1989)

Online resources

The instructor will mention several online resources during teaching.

How will the course be taught?

- 1 This course will be conducted in online mode completely. In case of any queries, please send an email to mainaks@iitk.ac.in

How will the course be taught?

- 1 This course will be conducted in online mode completely. In case of any queries, please send an email to mainaks@iitk.ac.in
- 2 All materials will be uploaded in mooKIT at least one week before the tutorial session. The students are encouraged to clarify doubts in the lecture materials during tutorial sessions.

How will the course be taught?

- 1 This course will be conducted in online mode completely. In case of any queries, please send an email to mainaks@iitk.ac.in
- 2 All materials will be uploaded in mooKIT at least one week before the tutorial session. The students are encouraged to clarify doubts in the lecture materials during tutorial sessions.
- 3 All in-course evaluations (in-video question plus quizzes) will be organized in the mooKIT

How will the course be taught?

- 1 This course will be conducted in online mode completely. In case of any queries, please send an email to mainaks@iitk.ac.in
- 2 All materials will be uploaded in mooKIT at least one week before the tutorial session. The students are encouraged to clarify doubts in the lecture materials during tutorial sessions.
- 3 All in-course evaluations (in-video question plus quizzes) will be organized in the mooKIT
- 4 Unless mentioned otherwise, the live tutorial will be organized through Zoom. However, it may change depending on the situations and we will follow accordingly. Such changes will be notified in advance. Further informations will be sent through the course alias emails.

Office: Office 4, C' block, Old-SAC complex

Email: mainaks@iitk.ac.in

Phone: 0512-259-2062

Homepage: <http://home.iitk.ac.in/~mainaks>

The students are very much encouraged to contact the instructor whenever needed