



INDIAN INSTITUTE OF TECHNOLOGY TIRUPATI

भारतीय प्रौद्योगिकी संस्थान तिरुपति

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|     |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                              |                                            |
|-----|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|--------------------------------------------|
| 1.  | Title of the course                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                          | Many-body theories of electron correlation |
| 2.  | Course number                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                | PH614L                                     |
| 3.  | Structure of credits (L-T-P-C)                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               | 3-0-0-3                                    |
| 4.  | New course/modification to                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   | New                                        |
| 5.  | To be offered by                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                             | Physics                                    |
| 6.  | Prerequisite                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                 | CoT                                        |
| 7.  | <b>Course Objective(s):</b> To outline basic concepts of many-particle quantum systems and their applications to the theory of quantum computing and quantum algorithm.                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      |                                            |
| 8.  | <b>Course Content:</b> Basic concepts in many-particle quantum systems: indistinguishability of identical particles, permutation symmetry, bosons and fermions; Mean-field theory: Hartree-Fock formalism, Brillouin's theorem, Koopmans' theorem, beyond mean field model, configuration interaction, wave operator, Bloch equation; Many-body perturbation theory: occupation number representation, creation and annihilation operators, Wick's theorem, diagrammatics; Coupled cluster theory: size extensivity, similarity, unitary transformed coupled cluster methods; Coupled cluster theory in quantum computing: variational quantum eigen solver algorithm, quantum equation of motion algorithm. |                                            |
| 9.  | <b>Textbook(s):</b><br>1. Crawford T D and Schaefer III H F, <i>An Introduction to Coupled Cluster Theory for Computational Chemists</i> , John Wiley and Sons, Ltd (2000).<br>2. Norman P, Ruud K, and Saue T, <i>Principles and Practices of Molecular Properties: Theory, Modeling, and Simulations</i> , Wiley (2018).                                                                                                                                                                                                                                                                                                                                                                                   |                                            |
| 10. | <b>Reference(s):</b><br>1. Shavitt I and Bartlett R J, <i>Many-body methods in Chemistry and Physics</i> , Cambridge University Press (2010).                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                |                                            |