

Experts

Prof. Yoshiyuki Kawazoe, Tohoku University, Japan

Prof. G. P. Das, Indian Association for the cultivation of Science, India

Dr. Ranjit Thapa, SRM Research Institute, India

(10 times x 1.15hrs)

1st day 3rd July - 10:00 A.M to 12:30 P.M

1. General Introduction ... Prof. Kawazoe

History in Computational Science; Two Big Users=Hydrodynamics(Finite Element Method) and *Ab Initio* Calculation(Density Functional Theory), Mathematical Complexities, Hardware Development(No Clock Speed Increment), Software Development, Original Software(Research=What you can do, others cannot), Commercialized Software, Classical and Quantum Mechanics, Electron is a Particle (Wave=Observation Problem)

2. Mathematical basics... Prof. Kawazoe

Solving Many Body Problem; Reduced Mass, Three-body Problem, Computational Accuracy, Propagation of Error, Theoretical Formulation for New Subjects, Fractals, Chaos, Large-scale Simulation, Parallel Computing

2nd day – 4th July – 10:00 A.M to 12:30 P.M

3. Introduction to CMS... Prof. G. P. Das

Computational Materials Science, Goals and Approach, Basic Procedure of Computational Materials Science Finite Element Analysis (FEA), Monte Carlo Methods, Schrödinger's Wave Equation, Energy Operator: Hamiltonian \hat{H} , Plane Wave, Standing Wave, Superposition Principles of Waves, Indistinguishability of Electrons, Infinite and Finite Well Problems, Hydrogen Atom, Degenerate States.

4. First-Principles Methods... Dr. Ranjit

Born–Oppenheimer (BO) Approximation, n-Electron Problem, Hartree Method: One-electron Model, Hartree-Fock Method: Expression for $\Psi(r)$, Orthogonality of Wave Functions, Expression for E, Variational Principles, Variational Approach to the Search for the Ground-state Energy, Self-Consistent Procedure, First-Principles Methods.

3rd day – 5th July - 10:00 A.M to 12:30 P.M

3. Density Functional Theory – I... Prof. G. P. Das

Reduced Density Matrices; Gilbert Theorem; Role of electron density; The problem of v-representability and N-representability; Hohenberg-Kohn Theorems; Kohn-Sham (KS) Equation; KS Orbitals & KS Eigenvalues;

4. Density Functional Theory – II... G. P. Das

Exchange-Correlation (XC) Hole; Local Density Approximation (LDA); Generalized Gradient Approximation (GGA); Jacob's Ladder for improved XC Functional; Practical aspects of

solving KS Equations: Self-consistency, Iterative Diagonalization, DOS, Bands, Total Energy and other Properties, Spin-polarized DFT; Limitations and cautionary remarks in using DFT. Quasiparticle Representations, Quasiparticle System Replacing n-electron System, DFT for Excited States, Finite-temperature DFT, Time Dependent DFT

4th day – 6th July - 10:00 A.M to 12:30 P.M

7. Molecular Dynamics... Dr. Ranjit

Atomic Model in MD, Classical Mechanics, Molecular Dynamics, Pair Potentials, Embedded Atom Method Potentials, Tersoff Potential, Potential for Ionic Solids, N-atom System, Verlet Algorithm, Velocity Verlet Algorithm, Predictor-corrector Algorithm, Potential Cutoff, Periodic Boundary Conditions.

8. Applications ... Prof. Kawazoe

Penta-graphene(New Geometry, IPR is not Perfect), Macky-like Crystals(First Single-element 3D Topological Insulator), Rare-metal Extraction (Recycle, Rh Extraction), Hydrogen Storage Materials (Transport as Hydrates for Fuel Battery Car), Magnetostriction Materials (Energy Harvesting, Battery-less System)

5th day – 7th July - 10:00 A.M to 12:30 P.M

9. More than the Present Standards... Prof. Kawazoe

TOMBO(The Original Software with GW, TDDFT based on All-electron Formulation, Absolute Energy Value Estimation), More than DFT(Deep Understanding of Quantum Mechanics, Origin of Chemical Bonds, Origin of Magnetism), Shifting Data Accumulation from Europe+USA to Our Region(Materials Database, Journal Publications)

10. Summary and Future Studies... Prof. Kawazoe + Dr. Ranjit

Big Paradigm-shift will Happen (From Explanation of Experimental Observation to Prediction of New Materials, Theoretical Studies are Safe, and Low Cost than Experiment), Design of Environmentally Good Materials (Renewable Energy is Not Simply Good), Materials Informatics(Big Data, Data-crunching, IoT, AI, Automatic Driving), Big Change in Life Always Realized by New Materials(LCC=Food is Not the Reason but New Light Body Reduces Cost)