Key Concepts in ME 539 (AP 639) *Heat Transfer Physics*

Principles of Atomic-Level Description of Thermal Energy Storage–Transport–Transformation

- Four principal thermal energy carriers: phonon, electron (hole), fluid particle, and photon
- Particle, waves, wave packets, and quasi-particle behaviors and statistics of bosons, fermions, and classical particles
- Atomic (fine structure) scales and units
- Molecular orbitals, interatomic potential (Schrödinger equation *ab initio* calculations) and potential models
- Molecular dynamics (MD) simulations and MD scales
- Schrödinger equation and its solutions: harmonic oscillator, electron gas, and electron in hydrogen-like atoms
- Boltzmann transport equation (BTE), particle scattering (interaction), and BTE scales
- Scattering (interaction) rate kinetics and Fermi golden rule (FGR)
- Maxwell equations: electromagnetic (EM) wave equation and relation to photon
- Onsager coupled transport coefficients and theorems
- Stochastic particle dynamics and transport (Langevin equation)
- Green–Kubo (G–K) transport coefficients (fluctuation-dissipation correlations)
- Macroscopic conservation equations (energy, fluid dynamics, and elastic-solid mechanics) and scales

Phonon Energy Storage, Transport and Transformation Kinetics

- Lattice and its vibration (phonon dispersion, bandgap, and density of states)
- Phonon heat capacity (Debye model)
- Phonon BTE, mean free path, and thermal conductivity (Callaway model)
- Phonon scattering mechanisms and relaxation-time models
- Cahill–Pohl minimum thermal conductivity model
- Slack relation and structural metrics of high-temperature phonon conductivity
- Phonon conductivity from MD and G–K autocorrelation decay and conductivity decomposition
- Phonon boundary resistance (diffuse and specular) using photon treatment and Debye model
- Size effects: Superlattice effective phonon conductivity

Electron Energy Storage, Transport and Transformation Kinetics

- Electrons in solids, band structure, allowed states and bandgaps and band-structure models, effective mass
- Electron density of states and heat capacity of metals and semiconductors
- Electron BTE and thermoelectric transport properties for semiconductors and metals
- Electron–phonon (acoustic and optical) scattering rates (scattering) from FGR
- Electron scattering by impurities and their relaxation-time models
- Electric thermal conductivity of solids (Wiedemann–Franz relation)
- Thermoelectricity (Seebeck, Thomson, Peltier coefficients) and figure of merit Z_eT for metals and semiconductors
- Electron–phonon thermal nonequilibrium and cooling length
- Size effects: quantum well for improved Z_eT ; reduced electron–phonon scattering rate in quantum wells

Fluid Particle Energy Storage, Transport and Transformation Kinetics

- Gas and liquid heat capacity (energy partition function and quantum fluid-particle energies)
- BTE and Maxwell-Boltzmann statistics, collision rate, thermal speeds, relaxation time and mean free path
- Gas thermal conductivity from BTE
- Liquid thermal conductivity (random, localized fluid particle motion)
- Conductivity of suspended particles in liquid (Brownian motion and nanofluid conductivity)
- Gas particle interaction with surface (fluid flow regimes and accommodations and slips)
- Solid particle thermophoresis in gases
- Physical surface adsorption and desorption of gas molecules
- Fluid-flow regimes: molecular-flow, Knudsen-flow, and turbulent-flow structure and transport
- Thermal plasmas and electron-heavy species thermal nonequilibrium
- Size effects: gas thermal conductivity in narrow gaps; thermal creep (slip) flow in narrow gaps

Photon Energy Storage, Transport and Transformation Kinetics

- Photon gas (blackbody) emission and radiation intensity
- Laser and near-field emissions (bandwidth and direction)
- Photon absorption and emission (spontaneous and stimulated) in two-level electronic systems
- Photon BTE and photon (and phonon) Equation of Radiative Transfer (ERT)
- EM Wave versus particle treatment of radiation (including photon localization)
- Mechanisms of spectral absorption in solids based on FGR (including semiconductors and metals)
- Mechanisms of spectral absorption in gases based on FGR (vibrational bands)
- Near- and far-field emission and reciprocity with absorption
- Radiative and nonradiative (e.g., phonon emission) decays and quantum efficiency
- Photon–electron–phonon couplings and laser cooling of solids (FGR)
- Role of fluid-particle quantum energy in gas laser and laser cooling of gases
- Role of phonon in photovoltaics and extraction of hot electrons
- Size effects: near-field radiation heat transfer; photon energy confinement by near-field optical microscopy