

# Introduction to soft matter and molecular ferroelectric science

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We will review the basic aspects of properties of soft matter and ferroelectric compounds, models and theories used in interpretation of data obtained from commonly used complementary experimental techniques. We will focus on interactions between molecules (long-range and short-range ones) and how they influence on physicochemical properties of solid and liquid states. Using concepts arising from numerous models and theories, we will put a special attention to look for understanding origins of physical quantities and their behaviour in fields of external parameters (such as temperature, pressure, electric or magnetic field, mechanical stress, etc.).

This course will cover key topics from the basic understanding and characterisation of selected soft matter and ferroelectric phenomena:

1. General information about properties of soft matter and ferroelectric materials:
  - a. characteristic of metaphases – nematic, cholesteric, smectic, conformationally and orientationally disordered plastic crystal phases;
  - b. properties of isotropic liquid and (ordered) crystal phases;
  - c. features and differences between ferro-, ferri-, antiferro-, para-electric phases;
  - d. brief description of commonly used experimental techniques: adiabatic calorimetry, differential scanning calorimetry (DSC), polarizing microscopy (POM), broadband dielectric spectroscopy (BDS), Fourier Transform Infrared Spectroscopy (FT-IR), X-ray Diffraction (XRD), Neutron Scattering (NS) – Inelastic Incoherent NS (IINS) and QuasiElastic NS (QENS), Nuclear Magnetic Resonance (NMR).
2. Description of phase transitions according to Landau theory:
  - a. Gibbs free energy – definition, examples, equation;
  - b. What is the order parameter (spontaneous polarization, magnetization, density, viscosity, mechanical strain, etc.)?;
  - c. The first and the second order phase transitions;
  - d. The heat capacity and susceptibility;
  - e. Isomorphous phase transitions.
3. The second order (continuous) phase transitions:
  - a. The (classical) Landau model;
  - b. Ising, Heisenberg models (brief characterisation);
  - c. Pyroelectric and dielectric measurements – introduction;
  - d. Widom and Griffiths scaling hypothesis;
  - e. Coupling of order parameters (in classical and sophisticated models);
  - f. Application to MAPCB, MAPBB, TGS, DMACA ferroelectrics.
4. The first order (discontinuous) phase transitions:
  - a. The classical Landau and the Landau-de Gennes models;
  - b. Adiabatic calorimetry measurements – introduction;

- c. The specific heat behaviour in the vicinity of melting temperature;
  - d. Application to neoalcohols (2,2-DM-1-B, 2,3-DM-2-B, 3,3-DM-1-B, 3,3-DM-2-B).
5. The isomorphous phase transitions:
- a. The Landau model;
  - b. The order parameter and the specific heat dependences;
  - c. Application to some neohexanol isomers (2,2-DM-1-B, 3,3-DM-2-B), liquid crystal (3TCB) and ferroelectrics (MAPCB, MAPBB).
6. Dielectric response – theory and application:
- a. Models – Debye, Cole-Cole, Cole-Davidson, Havriliak-Negami, Dissado-Hill;
  - b. Relaxation time – Arrhenius and Vogel-Fulcher-Tammann dependences, differences between them, activation enthalpy, fragile parameter, etc.;
  - c. Application to liquid crystals (4ABO5\*, 4EOB, 5BBAA, 6BBAA), pharmaceutical materials (ETH, C12CHdiol, C13CHdiol, T12CHdiol, T13CHdiol), selected glass-forming liquids, etc.;
  - d. Supercooled disordered phases;
  - e. Glasses of disordered phases (structural and orientational glasses);
  - f. Scaling of dielectric response (Nagel scaling, Dendzik & Paluch scaling, Galazka scaling) – application, determination of long-range and short-range correlation coefficients, etc.;
  - g. Scaling of supercooled disordered phases – important results;
  - h. Application of scaling – originally proposed for dielectric response – to other physical quantities (proton spin – lattice interaction, complex electric modulus, complex admittance and impedance).
7. Electric conductivity and electric polarization of electrode:
- a. D.C. conductivity – introduction and interpretation;
  - b. A.C. conductivity – Jonscher power law;
  - c. Electric polarization of electrode – power law/laws, interpretation;
  - d. Examples and application to dielectric response of real substances.
8. Short description of other methods used in studies on properties of condensed phase:
- a. Comparison of NMR and BDS spectroscopic results;
  - b. IINS and QENS applied to some liquid crystal materials;
  - c. Description of textures with the use of POM technique;
  - d. Dynamic Mechanical Analysis (DMA) applied to mechanical characteristic of ceramics.

Representative examples of compounds that illustrate mentioned key points will range from rigid glass-forming molecules (one-phenyl-ring molecules) to long liquid crystal molecules, built of rigid core (two or three phenyl ring joined by functional group, as azo- (-N=N-), ester- (-C(=O)-O-), azoxy- (-N=N(=O)-), etc.) and flexible parts – alkyl or alkoxy chain/chains, from dielectric to ferroelectric. Basic concepts and state-of-the art will be highlighted in the course.