Appendix A. A general outline of the comprehensive course for chemistry undergraduates of the Novosibirsk State University "Introduction into solid-state chemistry" (available on-line as Supplementary Material only)

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<tr><th>Lectures (54 academic hours)</th><th>Practicals (54 academic hours)</th></tr>
<tr><td colspan="2">Introduction into crystal structures</td></tr>
<tr><td>1. Structures of elements. Interrelation between the electronic structure of an element and the crystal structure.</td><td rowspan="4">Interactive work with the ICSD, CSDB, PDB databases using Mercury, Diamond, and PowderCell, CrystMet: retrieving structures, visualizing the structures, analyzing intramolecular geometry and intermolecular interactions, describing structures as close packings, as a set of polyhedra, in terms of hydrogen-bonded motifs (organic);

Discussion of structure-properties relations using selected examples.</td></tr>
<tr><td>2. Structures of compounds. How often do we deal with “inorganic molecules”?</td></tr>
<tr><td>3. Structures of organic crystals. Chemical bonds and non-covalent interactions.</td></tr>
<tr><td>4. Chains, layers and 3D-networks in inorganic and organic structures. Framework structures.</td></tr>
<tr><td colspan="2">Symmetry and basic crystallographic concepts</td></tr>
<tr><td>5. Symmetry operations in crystals: translations, point symmetry operations (inversion, rotations, inverse rotations, mirror reflection), open operations (glide, screw rotations). Translation groups, point groups, space groups. Asymmetric unit. Marices, graphical symbols. Crystallographic coordinate systems.</td><td rowspan="3">Interactive work with models of crystal structures and with crystallographic software: finding symmetry elements, unit cells, finding space and point groups, crystal systems and crystal families for the selected crystal structures.

Deriving space groups from generators, Finding special and general positions, presenting them graphically and via a set of matrices. Finding sub-groups and super-groups. Analyzing the possible effect of introducing / freezing a disorder on the symmetry.

Interactive work with International Tables for Crystallography, and with the materials at Bilbao Server. Transitions from one crystallographic setting to another. CIF generation.</td></tr>
<tr><td>6. Systematics of Bravais lattices, point groups, space groups. Crystal systems and crystal families. Nomenclature. Standard and non-standard settings. International Tables for Crystallography.</td></tr>
<tr><td>7. Non-crystalline solids. Commensurately and incommensurately modulated structures. Quasicrystals.</td></tr>
<tr><td colspan="2">Symmetry as a tool to predict properties</td></tr>
<tr><td>8. A physical property. Scalars, vectors, tensors of higher ranks. Curie and Neumann's principles.</td><td rowspan="3">Training on the application of Neumann's principle. Prediction of point groups which are not compatible with a particular property. Prediction of the allowed anisotropy of structure response to a particular external action for crystal structures belonging to various crystal systems.

Interactive work with the crystal structures of important materials, in order to correlate the structures with properties.

Training with model 1D and 2D examples: crystal orbitals, Bloch functions, E(k) diagrams, COOP functions, band filling. Peierls instability. Effects of doubling the unit cell. Effects of distorting symmetry. Interpretation of the energy band diagrams for selected 3D crystal structures.
Calculating the wavelength of light absorbed / emitted by a solid with a known energy band.
Predicting conductivity and its temperature dependence.</td></tr>
<tr><td>9. Structure response to variations in temperature, pressure, magnetic and electric fields, light</td></tr>
<tr><td>10. Structure-properties relationships. Examples of important materials. Interrelation between the anisotropy of properties and chemical interactions in inorganic and organic solids.</td></tr>
<tr><td>11. Symmetry of crystals and their electronic structure. Crystal orbitals. Energy bands. Metals, dielectrics, semiconductors. Pierls distortion. Energy gap tuning. Crystallographic symmetry and coordination chemistry. Modern materials.</td><td></td></tr>
<tr><td colspan="2">X-ray diffraction</td></tr>
<tr><td>12. A historical survey of studying crystal structures: before and after the X-rays have been discovered. Nobel prizes related to solution of crystal structures and developing the instruments and the calculation algorithms.</td><td rowspan="2">Exercises on reciprocal lattice.

Exercises on calculating and refining cell parameters and finding crystal system and space symmetry group from diffraction patterns. Calculation of strain tensors from the variable-temperature / variable-pressure diffraction</td></tr>
<tr><td>13. X-ray diffraction. A comparison with optical</td></tr>
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diffraction. Location of the centres of diffraction maxima (reflections). Laue conditions. Reciprocal lattice. Ewald illustration. Bragg equation. Finding cell parameters and crystal system.	data; discussion of the results in relation to a) the Neumann's rule, b) the bonds and interactions in the crystal structure.
14. Form-factor. Structural amplitude. Analysis of space group symmetry. Systematically absent reflections. Indexing of single-crystal and powder diffraction patterns. Absorption of X-rays by the sample. Intensity of reflections. Shape of reflections.	Indexing of powder diffraction patterns for the cubic system (manual). Indexing of powder diffraction patterns for lower-symmetry crystal systems (using software). The effect on the indices of a change in the crystallographic setting.
15. Calculating a diffraction patter for known structure. Refinement of crystal structures. Validation of the quality of structure solution and refinement. Origin of possible errors. Indications at possible errors. Solution of the unknown crystal structures. A general introduction into the direct methods. Origin of possible errors.	Absorption of X-rays by the sample. Calculating the absorption correction for a single crystal (using software). Calculating a diffraction patter for known structure using software. Predicting changes in the pattern resulting from: a) structure distortion, b) substitution of some species in the structure for the other, c) freezing / unfreezing of disorder.
16. The main variants of diffraction techniques. Samples. Radiation sources. Sample environment. The problems which can be solved by diffraction techniques. Equipment. Powder diffraction databases.	Suggesting an optimum strategy for sample preparation and data collection, aimed at solving a particular problem. Validation of the results of structure solution and refinement. Qualitative and quantitative analysis of the powder samples (individual phases and multiphase systems) using PDF database from the ICDD.
Real crystals – different types of defects	
17. Classification of defects. Equilibrium and non-equilibrium defects. Point defects. Linear defects. 2D and 3D defects. Impurities homogeneous / heterogeneous. Origin of defects in crystals. Quenching and annealing. Point defects. Kröger symbols. Quasi-chemical equations. Effect of impurities on the concentration of point defects. Non-stoichiometry. Point defects in semi-conductors and their properties.	Solving problems on calculating the concentrations of point defects under different conditions. Solving problems on the conductivity of semi-conductors. Solving problems on the interrelation between the concentration of point defects, impurities and non-stoichiometry.
18. Diffusion. Fick's laws. Einstein equation. Diffusion in the gradient of concentration, in the electric field, in the mechanical stress field. Ionic conductivity. Thermodynamic parameters characterizing point defects determined from conductivity measurements.	Calculating diffusion paths from diffusion coefficients. Solving problems on diffusion in the mechanical stress field. Calculating the free energy of defects formation, defects mobility and concentration from the results of the electrophysical measurements.
19. Fast ionic conductors. Materials for batteries, fuel cells, sensors. Interrelation between crystal structure and ionic conductivity. Conductivity of heterogeneous nanocomposites.	Analysis of the crystal structures of ionic conductors in relation to conductivity.
20. Clusters of point defects. F-centers. Optical properties of solids and point defects. Non-stoichiometry and "shear structures".	Analysis of clusters of point defects in relation to the crystal structures.
21. Dislocations. Disclinations. Stacking faults. External and internal surfaces. Mechanical properties of solids.	Analysis of dislocations and mechanical properties in relation to crystal structures.
22. Size effects in solid-state chemistry. Nanomaterials.	
23. Composite materials.	
24. Experimental techniques for studying size distribution of particles in a polycrystalline sample, strain, and extended defects. The methods of studying surfaces and extended defects in solids: diffraction, optical microscopy, electron microscopy, AFM.	Calculation of the coherent scattering domains from an experimental powder diffraction pattern. A comparison with the data on the particle size distribution in the same sample from microscopy data. Analysis of extended defects in a sample from powder diffraction data and electron microscopy data.

General overview (reactivity of solids)	
25. Reactivity of solids. Reactions within a solid; thermal decomposition.	A general discussion of selected solid-state properties and processes in as many aspects as possible. Refereeing published papers on "hot topics".
26. Reactivity of solids. Solid + solid, solid + liquid, solid + gas reactions.	
27. Concluding remarks. What is special with structures, properties, chemical reactions of solids? Properties depending on a) ideal structure, b) defects, c) the size / shape of a single crystal, d) the meso-structure (of the surface or of the bulk of the sample).	