# Glossary

**Artificial intelligence** is the ability of a machine to perform a task that would usually require the natural intelligence displayed by humans or animals.

**Axiom** is a statement that is taken to be true, to serve as a premise or starting point for further reasoning and arguments**.**

**Bioactivity** is an effect on, interaction with or response from a living tissue or cell.

**Biocompatibility** is the ability of a material to perform its function with an appropriate host response without causing any undesirable local and systemic effects.

**Biodegradation** is the mechanical, physical and chemical modification of a material by a biological environment and associated cells to break it down to its monomeric form.

**Biological assay** is an analytical method to determine the concentration or potency of a substance by its effect on living animals or plants (in vivo), or on living cells or tissues (in vitro).

**Biological environments** are cellular and physical surroundings of an organism, includes the factors that have an influence in their survival, development, and evolution.

B**iological molecules** is a term for molecules present in organisms that are essential for one or more biological processes, such as cell division, morphogenesis, or development.

**Black-box model** isa system which can be viewed in terms of its inputs and outputs (or transfer characteristics), without any knowledge of its internal workings.

**Cell phenotype** is the set of observable characteristics or traits of a cell.

**Chemical design space** is the property space spanned by all possible molecules and chemical compounds adhering to a given set of construction principles and boundary conditions.

**Chemical diversity** is the variety of chemical compounds present in an environment.

**Chemical resolution** is the degree of detail that can be achieved in measuring differences between molecules in an environment.

**Cross-validation** is a model validation technique for assessing how the results of a statistical analysis will generalize to an independent data set.

**Descriptors** arewords or features that serve to describe or identify something.

**Design of Experiments** is an organized method to study the relationship between multiple input variables and key output variables.

**Empirical statistical** (method) is used to describe and summarize empirical data in a convenient way.

**False negative** is an error where the test result incorrectly indicates the absence of a condition when it is present. Example: An individual is diagnosed negative for diabetes when they have the disease.

**False positive** is an error where the test result incorrectly indicates the presence of a condition (such as a disease when the disease is not present).

**Finite element method** isa widely used method for numerically solving differential equations arising in engineering and mathematical modelling.

**Full factorial design** is an experiment design where all the levels of all the factors are combined with one another. For example, if there are 2 factors, and each factor has 3 levels, then all possible combinations to perform the experiment is 23 = 8.

**Genetic methods (materials design)** are iterative approaches to materials design where materials are repeatedly synthesized, tested and then slightly modified in order to optimize the structure of a material for a particular performance criterion.

**Hidden layer** isa layer in between input and output layers in a neural network, where artificial neurons take in a set of weighted inputs and produce an output through an activation function.

**Homopolymer** is a chain of chemically linked molecules that are identical to each other.

**In vitro** meansstudies performed with microorganisms, cells, or biological molecules outside their normal biological context.

**In vivo** means studies in which the effects of various biological entities are tested on whole, living organisms or cells, usually animals, including humans, and plants.

**Input data** is the first set of data that a neural network uses to make a prediction.

**Kernel methods** area class of algorithms for pattern analysis with the general task to find and study general types of relations (for example clusters, rankings, principal components, correlations, classifications) in datasets.

**Locally optimal properties** are conditions where small increases or decreases to a material’s properties do not improve the material’s performance even though the conditions do not achieve the optimal performance.

**Machine learning methods** are approaches where a computer is able to train itself to perform a task, including supervised/unsupervised learning and reinforcement learning.

**Material stiffness** is the measure of a material's ability to resist deformation when acted on by an external force.

**Materials design space** refers to all the possible different material formulations.

**Mechanical interaction** is the capacity of an object to influence the motion of another object.

**Model components** are the variables associated with the subject of a model and the processes that link the variables together.

**Molecular fingerprinting** is a method of encoding the structure of a molecule in which a series of binary digits (bits) represents the presence or absence of particular substructures in the molecule.

**Nodes** are computational units that have one or more input connections. Input from the data is combined with a set of coefficients, that either increase or diminish it, thereby assigning significance to inputs according to the task the algorithm is trying to learn.

**Non-fouling** refers to the ability to resist the adsorption of biomolecules, such as proteins, or adhesion of cells.

**Nonlinear** isa system in which the change of the output is not linearly proportional to the change of the input.

**Ontologies** aredetailed formalizations of a certain area of ​​knowledge using a conceptual scheme. It consists of a data structure containing all relevant classes of objects and rules (theorems, restrictions) adopted in this area.

**Output layers** are the last layers thatproduce the final computational results in neural networks.

**Overfit** the production of an analysis that corresponds too closely or exactly to a particular set of data, and may therefore fail to fit additional data or predict future observations reliably

**Partial factorial design** consists of a carefully chosen subset of the experimental runs of a full factorial design.

**Physicochemical** involves both physical and chemical properties of a substance.

**Predictivity** isa condition when it is possible to accurately forecast future states of the system.

**Provenance** isa detailed record of model organism origin and history, to preserve its scientific significance.

**Quantitative structure-property relationships** arerelationships between chemical structure and biological activity or chemical property of a biomaterial.

**Readout** is a visual record of the experiment.

**Regenerative medicine** deals with the process of replacing, engineering or regenerating human or animal cells, tissues or organs to restore or establish normal function.

**Robustness** isthe property of a model when its outputs and forecasts are consistently accurate.

**Self-oxidation** is the property of a substance to react with itself in the presence of oxygen.

**Structure-function relationship** is the reliance relationship between the physical and chemical properties of a material on its functional properties.

**Synergistic effects** are interactions or cooperation giving rise to a whole that is greater than the simple sum of its parts.

**Synthetic polymers** are human-made substances or materials consisting of very large molecules and composed of repeating units.

**Test set** isa data set used to provide an unbiased evaluation of a final model fit on the training data set. The test set is not used to create the model.

**Tissue engineering** is the design and fabrication of living replacement devices for surgical reconstruction and transplantation.

**Topography** is the architectural landscape of the surface of a (bio)material.

**Total data set** is a collection of analytical results for all required variables.

**Training set** is the data initially used to create a computational model.

**Transfer function** isthe ratio of the output of a system to the input of a system.

**White-box modelling is** an abstract representation of a complex system in terms of equations or rules and a description of the region (spatially and/or temporally) on which these rules are valid.

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