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Computer modeling of disordered crystals

For several reasons, the title families of compounds are of increasing interest for theoretical investigation of composition-structure-properties relations. For instance, their wide range practical applications and thermodynamic stability are closely related to possible defects in the structure such as doping, vacancies, and atomic site substitutions. Recently, we have developed several approaches intended to perform comprehensive modeling of the properties for cathode materials [1–3], solid electrolytes [4,5], and intermetallics containing Mackay clusters[6].

Within the current research, the machine learning approaches are discussed as a tool for comprehensive description, better interpretation, and further extension of the results obtained by means of density functional theory (DFT) modeling numerous (up to several thousand) entries of the compositional/configurational spaces (CCS) of the studied materials. For each group of substances, sets of the relevant and robust structural-topological descriptors allowing to set/train computational models and, subsequently, to reduce the complexity of the CCS to be modeled within DFT approaches are considered in connection with the experimental results.

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