MODELING THE TOXICITY OF METAL NANOMATERIALS BY THE MEANS OF RELATIONAL MACHINE LEARNING

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Abstract

The modern trend in risk assessment of engineered nanoparticles includes predictive modeling to optimize the cost of toxicity experiments. The number of costly measurements is minimized by employing toxicity predictions, based on the structure and properties of similar materials which have already been assessed. Unlike modeling the structure-activity relationship of chemicals or bulk-form materials, modeling the toxic activity of nanomaterials is a challenging task. The nanomaterials have a more complex structure which needs to be described. Beyond the chemical structure of base compounds, there are higher supramolecular structures which the particles are organized in. Next, each nanoparticle has its own ontological structure of properties. This structure defines the equipment, design and preparation of a particle together with its empirical characterization such as size, surface and electrochemical potential. Henceforth, we propose to employ relational learning in the nanomaterial toxicity modeling. Unlike conventional machine learning algorithms, which have mainly been used for the (nano)structure-activity relationship modeling, the relational methods use the first-order logic to describe the particle. This is more natural data representation than widely-used attribute vectors, as the data consist of highly structured characterized particles. Moreover, the relational approach enables to define key properties of a particle which have potential toxic effect. Based on this rule, a new particle is prepared and assessed to refine the current model. This should lead to the optimal toxicity experiments and production of particles safe by design.

Keywords: Toxicity modeling, metal oxides, nano-QSAR, machine learning, inductive logic programming

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