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# Modelling the interactions of advanced micro- and nanoparticles with novel entities

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# Chapter 7

# General Discussion

Assessing the ecological risks of novel entities is essential for the protection of human health and environmental health. When multiple novel entities act simultaneously on organisms, they often cause toxic responses that are quite different from the effects of a single novel entity. However, due to the complexities of interactions between multiple novel entities, progress in understanding their combined impacts remains slow. Most traditional assessments of chemical toxicity effects have relied on *in vivo* and *in vitro* tests of biological toxicity. Since novel entities (e.g., engineered nanoparticles, ENPs) exhibit a high degree of complexity in terms of physicochemical properties, quantum mechanical properties, and toxicological effects, their risk evaluation is gradually shifting to *in silico* approaches based on understanding of the toxicity mechanisms. In order to avoid testing each novel entity from scratch, there is an urgent need to develop a series of *in silico* models to predict the environmental fate and biotoxic effects of novel entities.

This thesis aims to reveal the mechanisms of interaction between micro- and nanoparticles (MNPs) and other novel entities, investigate the impact of such interactions on the environmental behavior and effects of novel entities, and assess and predict the combined toxicity of ENPs and other novel entities to ecological species. First, we investigated the interaction mechanisms between carbon-based nanoparticles (CNPs) and a severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2) ribonucleic acid (RNA) fragment and we developed quantitative structure-activity relationship (QSAR) models to predict this interaction. Second, we revealed the interaction mechanism between microplastics (MPs) and a SARS-CoV-2 RNA fragment and its influencing factors. Third, we clarified the modes of

action and influencing factors of the combined toxicity of multiple ENPs to ecological species. Finally, we developed QSAR models based on machine learning (ML) methods to predict the ecotoxicity of mixtures of binary metal oxide nanoparticles ($MO_X$ NPs).

## 7.1 Solved research questions and environmental implications

To achieve the aims described above, this thesis answered four questions to promote the understanding of the interaction between different novel entities and the impacts of the interaction on the environmental behavior and biological effects of novel entities.

### 7.1.1 Interaction and mechanisms of ENPs with SARS-CoV-2 macromolecules

We found that the interaction mechanism between CNPs and a SARS-CoV-2 RNA fragment is driven by electrostatic interactions through molecular mechanics simulation studies. Furthermore, we found that molecular weight, surface area, and the sum of degrees of every carbon atom as the primary structural descriptors determined the interaction between the CNPs and the SARS-CoV-2 RNA fragment. The above findings suggest that the interaction between CNPs and biomolecules mainly depends on the intrinsic properties of CNPs, especially their surface properties. CNPs have a high specific surface area, which leads to a large number of surface atoms or molecules that can interact with biomolecules.

At the same time, we found that the order of magnitude of the interaction force between the CNPs and the SARS-CoV-2 RNA fragment was: carbon nanotubes > graphene > fullerene. This also

indicates that the surface properties of CNPs are affected by various factors, such as size, shape, surface charge, hydrophobicity and chemical composition. For example, ENPs with a large surface area, high surface energy, and hydrophobicity tend to adsorb RNA and other biomolecules (e.g., proteins), leading to the formation of nanoparticle-RNA or -protein coronas on the surface of ENPs. Existing studies confirm that the formation of eco-coronas (Liu et al., 2023; Wheeler et al., 2021), represented by protein coronas, can alter the physicochemical properties of ENPs and affect their toxicity (Ekvall et al., 2021). Eco-coronas can reduce the surface charge and increase the hydrophilicity of ENPs, leading to changes in their cellular uptake, biodistribution and toxicity (Chakraborty et al., 2021; Diaz-Diestra et al., 2022). Eco-coronas may also modulate the interaction of ENPs with cell membranes and intracellular organelles (Feng et al., 2023; Liu et al., 2022), leading to alterations in their intracellular fate and toxicity.

In addition, such interactions may also have affected the structure or stability of viral RNA. In terms of viral migration and exposure, the interaction between ENPs and viral RNA may have positive effects. For example, ENPs may interfere with the ability of the virus to enter cells, replicate, or spread throughout the body (Bhatti and DeLong, 2023; Campos et al., 2020; Li et al., 2023). This may reduce the severity of infection or prevent it from occurring altogether. Furthermore, the effect of ENP-viral RNA interactions on viral migration and exposure would depend on the specific characteristics of the ENPs and the virus.

### 7.1.2 Interaction and mechanisms of MPs with SARS-CoV-2 macromolecules

We found that the interaction mechanism between MPs and SARS-CoV-2 RNA fragments involves electrostatic and hydrophobic processes through molecular dynamics simulation studies. Moreover, the affinity of the interaction was related to the intrinsic structural parameters of the MP monomer (i.e., molecular volume, polar surface area, and molecular topological index). It can be seen that the surface properties of MPs make biomolecules to attach to the surface of MPs. This also implies that MPs may be an important homing site for biomolecules. We also found that for the SARS-CoV-2, the interaction force between MPs and their RNA fragments was stronger than the interaction force between MPs and their nucleocapsid proteins. However, for the Hepatitis B virus (HBV), the MPs showed stronger interactions with the nucleocapsid protein than with its RNA fragment. This also suggests that the interaction between the MPs and the viral biomolecules is closely related to the type of microorganism.

The interaction between MPs and biomolecules is a complex process that can have a range of impacts on their environmental behavior and biological toxicity (Junaid and Wang, 2022; Luo et al., 2022). First, this interaction could alter the physical properties of MPs, such as surface charge, hydrophobicity, and aggregation, leading to changes in their transport and distribution in the environment. Second, the adsorption of biomolecules on MPs could affect their biological interactions with organisms. For example, the adsorption of proteins on MPs can alter the bioavailability and toxicity of MPs to organisms (Cao et al., 2022). Finally, the adsorption of biomacromolecules on

MPs could affect the fate and persistence of MPs in the environment, similar to nanomaterials (Lowry et al., 2012). MPs with adsorbed biomacromolecules may be more resistant to degradation and biofouling, making their long-term persistence in the environment more likely. Thereupon, understanding the mechanisms of interaction between MPs and biomolecules is essential for developing effective strategies to mitigate their environmental impacts and protect human and ecological health.

Currently, viral infections remain a major public health concern and the potential role of MPs in facilitating virus transmission and exposure is an area of active research. The small size of MPs may allow them to serve as carriers for transporting viral particles (Lu et al., 2022; Zhai et al., 2023). For instance, a recent study found that MPs in wastewater can carry SARS-CoV-2 (Belišová et al., 2022). This thesis also found that the high surface area of MPs and their ability to adsorb the biomolecules of SARS-CoV-2 may make them effective carriers of viral particles.

The effect of MPs on virual transmission and exposure may also depend on environmental factors. The present findings in this thesis reveal that MPs interact stronger with viral RNA fragments in an aqueous environment than in the gas phase. Previous studies have also found that the presence of MPs in water may increase the likelihood of virus particles surviving and remaining infectious (Amato-Lourenço et al., 2022; Moresco et al., 2021), but MPs may also decrease the concentration in air of virus particles by adsorbing them to the MP surface. The interaction of MPs with viral RNA may also be influenced by a range of other environmental factors, including temperature, pH, and the presence of other contaminants.

### 7.1.3 Joint interactions after exposure of ecological test species to multiple ENPs and factors determining the toxicity of a mixture of multiple ENPs

When multiple novel entities are present in the environment, they exert effects on ecological species (including algae, bacteria, Daphnia, fish, fungi, insects and plants) via different modes of action. Taking mixtures of multiple ENPs as an example, we found that in studies specifying the combined toxic response of mixtures of ENPs, 53 % showed antagonistic effects, 25 % synergistic effects, and 22 % additive effects. From this result, it is clear that the interactions between multiple ENPs are mainly antagonistic. This implies that if multiple ENPs coexist in the environment, their combined effects on ecological species will be smaller than the effects when each of them is present alone. However, the synergistic effects exhibited among multiple ENPs cannot be ignored. The synergistic effects occur so that the presence of multiple ENPs can have a greater effect on ecological species compared to exposure to each pollutant individually.

The combined toxic effects of multiple novel entities on ecological species depend on many factors. This thesis reveals that the main factors influencing the type of combined toxic response of biota to exposure to mixtures of ENPs are 1) the chemical composition of the individual components of the mixture, 2) the stability of the suspension of mixed ENPs, 3) the type and trophic level of the individual organisms tested, 4) the level of biological organization (population, community, and ecosystem), 5) the exposure concentration and exposure duration, 6) the toxicity endpoints, and 7) abiotic scenario conditions (e.g., pH, ionic strength, natural organic matter).

Specifically, different combinations of ENPs have different toxic effects on ecological species, and their joint effects may be influenced by their exposure concentrations in the environment. The concentration of a mixture component may be influenced by the source of the ENP mixtures and the environmental conditions which affect their distribution and transport (Buzea et al., 2007). Another factor that affects the joint toxic effects of multiple ENPs is the exposure pathway. Ecological species can be effectively exposed to mixtures of ENPs through a variety of routes, such as inhalation, ingestion, and dermal contact. Exposure routes affect the toxicity levels of mixtures of ENPs and the extent of their effects on ecological species. Duration of exposure is one factor that affects the toxic effects of multiple ENPs. Short-term exposure to mixtures of ENPs can have different effects on ecological species compared to long-term exposure (Jośko et al., 2022). Long-term exposure to low levels of ENPs can lead to chronic toxicity that may not be immediately apparent, but can have cumulative effects over time. The sensitivity of ecological species to mixtures of ENPs is also an important factor affecting their joint toxic effects. Additionally, environmental conditions, such as temperature, pH, and solution parameters, can also affect the distribution and transport of ENPs in the environment, as well as their persistence and bioavailability, and thus their joint effects on ecological species. Understanding the interactions of multiple ENPs and their joint toxic effects is critical to developing effective strategies to prevent and mitigate pollution and to protect the environment and ecological species.

### 7.1.4 Development of QSAR models based on ML approaches for predicting the mixture toxicity of multiple ENPs

In this thesis, a ML-based QSAR method was established to quantitatively predict the cytotoxicity of a mixture of binary ENPs against *Escherichia coli*, using $MO_X$ NPs as a case. The QSAR model based on support vector machine and neural network methods was found to exhibit good predictive power for both the constructed internal dataset and the combined internal and external datasets. It is thus seen that the combination of ML and QSAR methods provides several advantages for predicting the toxicity of ENPs. These include:

1) Accurate predictions: ML models can identify complex relationships between nanostructure and toxicity, which can lead to more accurate toxicity predictions than traditional QSAR models.

2) Improved efficiency: ML models can analyze datasets quickly and efficiently, saving time and resources compared to traditional QSAR modeling.

3) Ability to handle large data: With the rapid growth of nano-toxicological data, ML techniques can effectively handle large and complex datasets with high dimensionality.

4) Generalizability: ML models can learn patterns from a large number of different nanostructures, making them more generalizable to new ENPs.

5) Flexible modeling: ML models can be tailored to specific toxicological endpoints and can handle complex nonlinear relationships, allowing the development of models that can predict a

wide range of toxicological endpoints.

However, there are still areas for improvement in ML-based QSAR models used to predict the toxicity of ENPs. Some of these areas include:

1) Data quality: The quality and reliability of the nanotoxicological data used to develop and validate ML models are critical to their accuracy and reliability. Further improvements in data quality are necessary to ensure the validity and reproducibility of these models.

2) Interpretability: The interpretation of ML models can be challenging and complex, which may limit their utility in regulatory decision making. Developing methods to improve the interpretability of these models is thus critical.

3) Nanostructure diversity: Many ML models are based on a relatively small subset of nanostructures. More studies are required to ensure that these models can accurately predict the toxicity of a broader range of nanostructures. Consequently, further work is needed to demonstrate the reliability and robustness of these models for use in regulatory decision making.

In short, methodologies for assessing and predicting the mixture toxicity of multiple novel entities are lagging far behind the rapid emergence of new chemicals. Big data, deep learning, and artificial intelligence present unprecedented opportunities and challenges for assessing the toxicity of mixtures of novel entities. The models developed in this thesis show that our research approach can provide a methodological and theoretical basis for ecological risk assessment

of mixtures of novel entities.

## 7.2 Future risk and hazard assessment of novel entities and their mixtures

### 7.2.1 Ecological risk assessment of multiple novel entities

Today, scientists recognize that novel entities require global environmental attention because the majority of man-made chemical "novel entities" have been reported to enter the environment and most likely in future MNPs have the potential for lasting impact, large-scale distribution, and influence on important Earth system processes. Advances in synthesizing MNPs is also occurring at a rapid pace. Therefore, risk assessment of novel entities is a critical step in ensuring the safety of chemical products, the environment and public health. It involves identifying, assessing, and quantifying the potential risks posed by chemical substances present in a variety of environments, such as water, air, and soil. The risk assessment process for novel entities could learn from the traditional chemical risk assessment process (Van Leeuwen et al., 1996), which comprises of the stages listed below:

1) Hazard identification: The potential hazards associated with chemicals are identified and described. This involves the collection and analysis of data on toxicity, exposure, and other relevant factors that might have negative health consequences.

The general paradigm of comparing exposure to hazards, also applies to novel entities albeit that it is essential to base hazard and exposure on the same metrics of exposure (number, surface area, mass concentration, etc.).

2) Exposure assessment: The extent and frequency of exposure to chemicals in the environment or related products are determined. This involves collecting data on sources, routes, and levels of exposure.

The classical chemicals are usually dealt with homogeneous solutions. However, in case of novel entities such as ENPs and MPs, we often deal with non-stable suspensions. This requires a different approach to assessment of the effective exposure and the assessment of bioavailability of the novel entities.

3) Dose-effect assessment: The relationship between the exposure dose of chemicals and their adverse health effects is assessed. This involves assessing toxicological data and establishing dose-effect relationships.

In addition to the exposure dose or concentration, the physicochemical properties (particle size, surface charge, etc.) of novel entities such as ENPs and MPs have a significant impact on their toxic effects on ecological species. Therefore, establishing the relationship between the physicochemical properties of novel entities and their effects would help to determine their biological toxicity quickly. Besides, the toxic effects of novel entities are also closely related to abiotic factors (pH, divalent cations, natural organic matter, etc.). Thereupon, the impacts of abiotic factors need to be considered when establishing the dose/concentration-effect relationships of novel entities.

4) Risk characterization: The information gathered in the previous steps to assess the overall risk posed by the chemicals is integrated. This includes assessing the likelihood and severity of

adverse effects and determining appropriate risk management measures.

A series of assessment standards and rules, index parameters, testing tools and methods for the risk management of novel entities need to be proposed. Furthermore, advanced analytical and testing technologies combined with *in silico* methods need to be used for detection, exposure assessment, hazard and risk identification of novel entities.

How to implement a scientific, systematic and comprehensive risk assessment of novel entities is an important topic for future environmental toxicology research. A powerful and extremely practical strategy for accelerating the evaluation process is the establishment of reliable assessment procedures. Moreover, essential information on risk management measures would be provided, including setting exposure limits, establishing regulations, and implementing control measures.

### 7.2.2 Developments in toxicity prediction for novel entities and their mixtures

The novel entities in the environment are diverse in nature and are associated with complex distribution patterns, bringing about complex ecological and environmental health effects. With the advancement of modern society and global economy, new chemicals are constantly produced and applied, and inevitably constantly released into the environment. The novel entities released into the environment are in the form of mixtures of monomers or complexes, and there are complex interactions between different novel entities such as antagonism and synergism. The study of the biological

activities of different combinations of novel entities and their joint effects is a difficult and hot research area for the international environmental science community. Therefore, the complex effects of the coexistence of multiple novel entities bring new opportunities and new challenges to environmental health research.

***Development of advanced prediction methods***

Chemical toxicity prediction is an important task in the fields of drug discovery, environmental protection and public health (Alves et al., 2018; Pérez Santín et al., 2021). To date, advanced methods for chemical toxicity prediction are emerging, such as QSAR models (Chen et al., 2017), ML models (Balraadjsing et al., 2022), and deep learning models (M. Xu et al., 2022), which can not only analyze the chemical structures of compounds but also predict their toxicity with high accuracy. These methods are based on the principle that the molecular structural characteristics of a chemical determine its biological activity, including its toxicity.

Advanced *in silico* methods for chemical toxicity prediction have the potential to revolutionize the field of toxicology. *In silico* predictions have the ability to handle large and complex datasets. Moreover, in contrast to traditional component-based toxicity prediction methods, *in silico* methods can provide accurate and interpretable chemical toxicity predictions that can help researchers and policy makers to make informed decisions about the safety of chemicals. More importantly, *in silico* methods can provide insight into the molecular properties that contribute to chemical toxicity. This information can be used to design safer and more effective drugs or chemicals.

For the purpose of environmental risk management of novel entities

and their mixtures, future research can develop classification and cross-comparison analogy techniques for novel entities and their mixtures by using ML algorithms such as classification-based fuzzy clustering, decision trees, and support vector machines. Meanwhile, further research can develop QSAR models for toxicity prediction of novel entities and their mixtures by utlizing nanostructure-based molecular mechanics/dynamics, Monte Carlo, quantum chemistry, and other molecular simulation methods. A complete system of intelligent detection strategies for ecotoxicological risk assessment of novel entities (including mixtures) is likely to be established in future by using *in silico* methods.

### *Constructing a toxicity prediction platform*

Screening and assessing the toxicity effects of emerging novel entities as they are identified, is important to avoid the release of high-risk novel entities into the environment to produce more serious hazards. To quickly and accurately determine the biological toxicity effects of novel entities and their mixtures, it is necessary to develop a computer-based platform for predicting the environmental behavior and toxicity of novel entities (Figure 7.1).

The establishment of a toxicity prediction platform for novel entities (including mixtures) involves the development of a system that can accurately predict the toxicity of novel entities based on their molecular structure and properties. With the use of this platform, it is possible to evaluate any risks that could come with exposure to novel entities and to identify safer alternatives for use in various industries, including pharmaceuticals, agriculture, and consumer products. As an example of the process of building a mixture toxicity prediction

platform for multiple novel entities, the platform building process consists of the following:

1) Data collection: A process of collecting a great deal of data on the chemical structure and properties of various novel entities, as well as information on their single and combined toxic effects. These data can be obtained from various sources, including experimental studies, toxicological databases, and published literature.

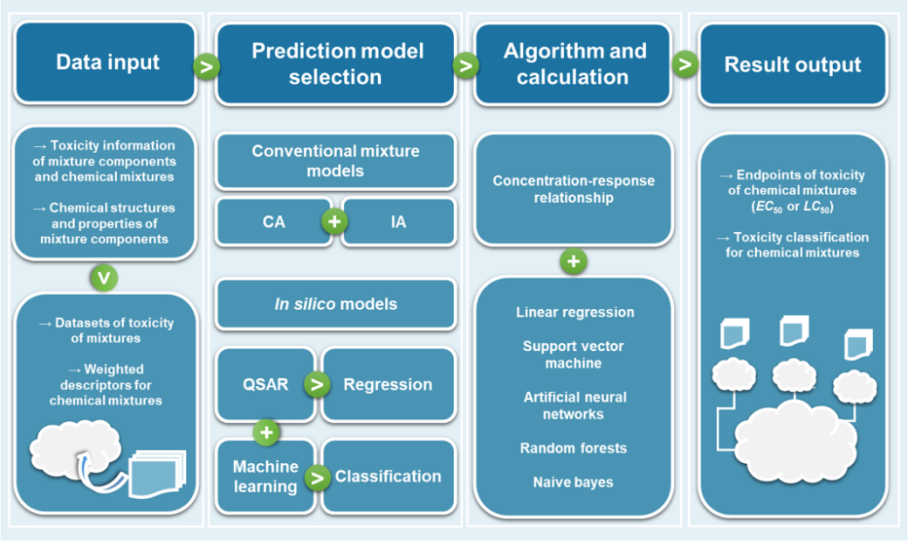


***Figure 7.1.*** *Schematic diagram of the construction of a toxicity prediction platform for novel entities and their mixtures.*

2) Predictive model selection: Based on the completeness and richness of the collected toxicity data of mixtures of novel entities, the basic methodologies for building predictive models are selected, i.e., traditional mixture models based on mixed components and QSAR and ML models based on computational methods.

3) Predictive model development and validation: Analysis with computational methods to identify patterns and associations between

chemical structure and toxicity is carried out. This analysis typically includes the use of ML algorithms that are trained on the collected data to develop predictive models that accurately predict the toxicity of novel entities based on their molecular structures and properties. These predictive models are then validated using additional experimental data to ensure that they are accurate and reliable. This validation process typically involves comparing the predicted toxicity of the novel entities with the actual toxic effects measured in laboratory studies. To improve the accuracy and reliability of the predictive models, additional data can be included in the analysis, including information on the metabolic pathways and biological targets of the novel entities, as well as their physical and chemical properties.

4) The output of results: Once the predictive models have been validated, they can be integrated into a user-friendly platform that researchers and industry experts can use to evaluate the toxicity of the novel entities and to identify safer alternatives. This platform could include various features such as a user-friendly interface, customizable search capabilities, and interactive visualization tools.

To sum up, building a toxicity prediction platform for novel entities (including mixtures) requires a multidisciplinary approach that combines expertise in chemistry, toxicology, computational methods, and data analysis. By accurately predicting the toxicity of novel entities (including mixtures), the constructed platform can help reduce the single and joint risks associated with exposure to hazardous novel entities and promote the development of safer and more sustainable chemical products. This thesis brings the scientific community as a well as policymakers and industrial stakeholders new

information such as theoretical models and computational simulations were used to combine cytotoxicity experiments and data to understand and predict interactions between MNPs and novel entities. Within the thesis the interaction of MNPs of different dimensions with the SARS-CoV-2 RNA fragment only was investigated, but it can be used as a reference for exploring the interaction of MNPs with other RNA-based fragments. Similarly the work on the mixture and interaction models developed for metallic ENPs would also be the basis for the modeling of hybrid and other advanced metal-bearing ENPs.

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