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

Zhang, F.

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.

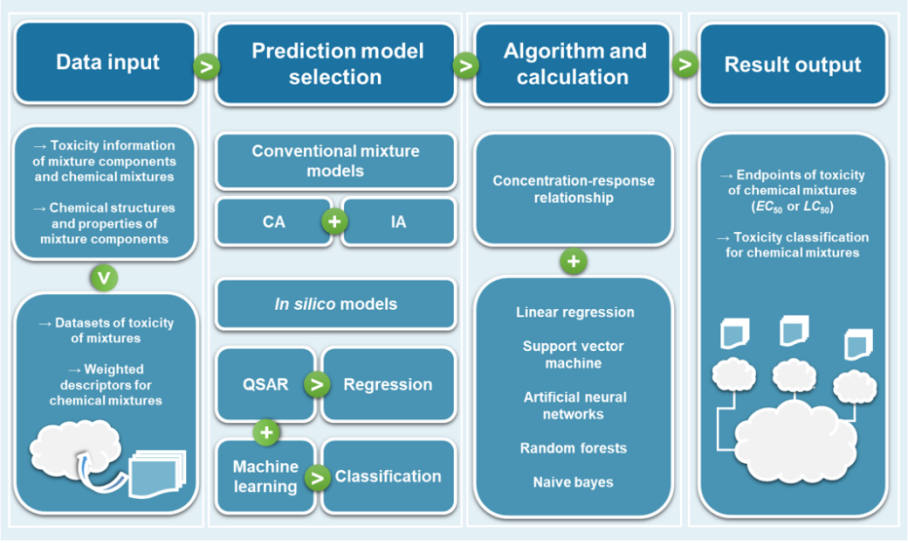

Figure 7.1. *Schematic diagram of the construction of a toxicity prediction platform for novel entities and their mixtures.*

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.

References

Aasi, A., Aghaei, S.M., Moore, M.D., Panchapakesan, B., 2020. Pt-, Rh-, Ru-, and Cu-single-wall carbon nanotubes are exceptional candidates for design of anti-viral surfaces: A theoretical study. Int. J. Mol. Sci. 21, 5211. https://doi.org/10.3390/ijms21155211.

Abbas, Q., Liu, G., Yousaf, B., Ali, M.U., Ullah, H., Ahmed, R., 2019. Effects of biochar on uptake, acquisition and translocation of silver nanoparticles in rice (*Oryza sativa* L.) in relation to growth, photosynthetic traits and nutrients displacement. Environ. Pollut. 250, 728–736. https://doi.org/10.1016/j.envpol.2019.04.083.

Abbas, Q., Yousaf, B., Amina, Ali, M.U., Munir, M.A.M., El-Naggar, A., Rinklebe, J., Naushad, M., 2020. Transformation pathways and fate of engineered nanoparticles (ENPs) in distinct interactive environmental compartments: A review. Environ. Int. 138, 105646. https://doi.org/10.1016/j.envint.2020.105646.

Aboubakr, H.A., Sharafeldin, T.A., Goyal, S.M., 2021. Stability of SARS-CoV-2 and other coronaviruses in the environment and on common touch surfaces and the influence of climatic conditions: A review. Transbound. Emerg. Dis. 68, 296–312. https://doi.org/10.1111/tbed.13707.

Achak, M., Alaoui Bakri, S., Chhiti, Y., M'hamdi Alaoui, F.E., Barka, N., Boumya, W., 2021. SARS-CoV-2 in hospital wastewater during outbreak of COVID-19: A review on detection, survival and disinfection technologies. Sci. Total Environ. 761, 143192. https://doi.org/10.1016/j.scitotenv.2020.143192.

Adelodun, B., Ajibade, F.O., Tiamiyu, A.O., Nwogwu, N.A., Ibrahim, R.G., Kumar, P., Kumar, V., Odey, G., Yadav, K.K., Khan, A.H., Cabral-Pinto, M.M.S., Kareem, K.Y., Bakare, H.O., Ajibade, T.F., Naveed, Q.N., Islam, S., Fadare, O.O., Choi, K.S., 2021a.

Monitoring the presence and persistence of SARS-CoV-2 in water-food-environmental compartments: State of the knowledge and research needs. Environ. Res. 200, 111373. https://doi.org/ 10.1016/j.envres.2021.111373.

Adelodun, B., Kareem, K.Y., Kumar, P., Kumar, V., Choi, K.S., Yadav, K.K., Yadav, A., El- Denglawey, A., Cabral-Pinto, M., Son, C.T., Krishnan, S., Khan, N.A., 2021b. Understanding the impacts of the COVID-19 pandemic on sustainable Agri-food system and agroecosystem decarbonization nexus: A review. J. Clean. Prod. 318, 128451. https://doi.org/10.1016/j.jclepro.2021.128451.

Ahmed, B., Khan, M.S., Musarrat, J., 2018. Toxicity assessment of metal oxide nano-pollutants on tomato (*Solanum lycopersicon*): A study on growth dynamics and plant cell death. Environ. Pollut. 240, 802–816. https://doi.org/10.1016/j.envpol.2018.05.015.

Ahmed, W., Bertsch, P.M., Bibby, K., Haramoto, E., Hewitt, J., Huygens, F., Gyawali, P., Korajkic, A., Riddell, S., Sherchan, S.P., Simpson, S.L., Sirikanchana, K., Symonds, E. M., Verhagen, R., Vasan, S.S., Kitajima, M., Bivins, A., 2020. Decay of SARS-CoV-2 and surrogate murine hepatitis virus RNA in untreated wastewater to inform application in wastewater-based epidemiology. Environ. Res. 191, 110092. https://doi.org/10. 1016/j.envres.2020.110092.

Al Huraimel, K., Alhosani, M., Kunhabdulla, S., Stietiya, M.H., 2020. SARS-CoV-2 in the environment: Modes of transmission, early detection and potential role of pollutions. Sci. Total Environ. 744, 140946. https://doi.org/10.1016/j.scitotenv.2020.140946.

Allawadhi, P., Khurana, A., Allwadhi, S., Joshi, K., Packirisamy, G., Bharani, K.K., 2020. Nanoceria as a possible agent for the management of COVID-19. Nano Today 35, 100982. https://doi. org/10.1016/j.nantod.2020.100982.

Allen, S., Allen, D., Baladima, F., Phoenix, V.R., Thomas, J.L., Le

Roux, G., Sonke, J.E., 2021. Evidence of free tropospheric and long-range transport of microplastic at Pic du Midi Observatory. Nat. Commun. 12, 7242. https://doi.org/10.1038/s41467-021-27454-7.

Almansour, N.A., Syed, H.F., Khayat, N.R., Altheeb, R.K., Juri, R.E., Alhiyafi, J., Alrashed, S., Olatunji, S.O., 2019. Neural network and support vector machine for the prediction of chronic kidney disease: A comparative study. Comput. Biol. Med. 109, 101–111. https://doi.org/10.1016/j.compbiomed.2019.04.017.

Altenburger, R., Nendza, M., Schüürmann, G., 2003. Mixture toxicity and its modeling by quantitative structure–activity relationships. Environ. Toxicol. Chem. 22, 1900–1915. https://doi.org/10.1897/01-386.

Alves, V.M., Muratov, E.N., Zakharov, A., Muratov, N.N., Andrade, C.H., Tropsha, A., 2018. Chemical toxicity prediction for major classes of industrial chemicals: Is it possible to develop universal models covering cosmetics, drugs, and pesticides? Food Chem. Toxicol. 112, 526–534. https://doi.org/10.1016/j.fct.2017.04.008.

Amato-Lourenço, L.F., de Souza Xavier Costa, N., Dantas, K.C., dos Santos Galvão, L., Moralles, F.N., Lombardi, S.C.F.S., Júnior, A.M., Lindoso, J.A.L., Ando, R.A., Lima, F.G., Carvalho-Oliveira, R., Mauad, T., 2022. Airborne microplastics and SARS-CoV-2 in total suspended particles in the area surrounding the largest medical centre in Latin America. Environ. Pollut. 292, 118299. https://doi.org/10.1016/j.envpol.2021.118299.

Amato-Lourenço, L.F., dos Santos Galvão, L., de Weger, L.A., Hiemstra, P.S., Vijver, M.G., Mauad, T., 2020. An emerging class of air pollutants: Potential effects of microplastics to respiratory human health? Sci. Total Environ. 749, 141676. https://doi.org/10.1016/j.scitotenv.2020.141676.

Anand, U., Bianco, F., Suresh, S., Tripathi, V., Núñez-Delgado, A., Race, M., 2021. SARS-CoV-2 and other viruses in soil: An environmental outlook. Environ. Res. 198, 111297. https://doi.org/10.1016/j.envres.2021.111297.

Anonymous, 2020. Nanotechnology versus coronavirus. Nat. Nanotechnol. 15, 617. https://doi.org/10.1038/s41565-020-0757-7.

Arp, H.P.H., Kühnel, D., Rummel, C., MacLeod, M., Potthoff, A., Reichelt, S., Rojo-Nieto, E., Schmitt-Jansen, M., Sonnenberg, J., Toorman, E., Jahnke, A., 2021. Weathering plastics as a planetary boundary threat: Exposure, fate, and hazards. Environ. Sci. Technol. 55, 7246–7255. https://doi.org/10.1021/acs.est.1c01512.

Arslan, M., Xu, B., Gamal El-Din, M., 2020. Transmission of SARS-CoV-2 via fecal-oral and aerosols-borne routes: Environmental dynamics and implications for wastewater management in underprivileged societies. Sci. Total Environ. 743, 140709. https://doi.org/10.1016/j.scitotenv.2020.140709.

Asher, C., 2021. Novel chemical entities: Are we sleepwalking through a planetary boundary? (mongabay.com)

Avellan, A., Yun, J., Morais, B.P., Clement, E.T., Rodrigues, S.M., Lowry, G.V., 2021. Critical review: Role of inorganic nanoparticle properties on their foliar uptake and *in planta* translocation. Environ. Sci. Technol. 55, 13417–13431. https://doi.org/10.1021/acs.est.1c00178.

Azevedo, S.L., Holz, T., Rodrigues, J., Monteiro, T., Costa, F.M., Soares, A.M.V.M., Loureiro, S., 2017. A mixture toxicity approach to predict the toxicity of Ag decorated ZnO nanomaterials. Sci. Total Environ. 579, 337–344. https://doi.org/10.1016/j.scitotenv.2016.11.095.

Azimzada, A., Jreije, I., Hadioui, M., Shaw, P., Farner, J.M.,

Wilkinson, K.J., 2021. Quantification and characterization of Ti-, Ce-, and Ag-nanoparticles in global surface waters and precipitation. Environ. Sci. Technol. 55, 9836–9844. https://doi.org/10.1021/acs.est. 1c00488.

Baek, M.J., Son, J., Park, J., Seol, Y., Sung, B., Kim, Y.J., 2020. Quantitative prediction of mixture toxicity of $AgNO_3$ and ZnO nanoparticles on *Daphnia magna*. Sci. Technol. Adv. Mater. 21, 333–345. https://doi.org/10.1080/14686996.2020.1766343.

Balraadjsing, S., Peijnenburg, W.J.G.M., Vijver, M.G., 2022. Exploring the potential of *in silico* machine learning tools for the prediction of acute *Daphnia magna* nanotoxicity. Chemosphere 307, 135930. https://doi.org/10.1016/j.chemosphere.2022. 135930.

Ban, M.J., Lee, D.H., Shin, S.W., Kim, K., Kim, S., Oa, S.-W., Kim, G.-H., Park, Y.-J., Jin, D.R., Lee, M., Kang, J.-H., 2022. Identifying the acute toxicity of contaminated sediments using machine learning models. Environ. Pollut. 312, 120086. https://doi.org/ 10.1016/j.envpol.2022.120086.

Barros, J., Seena, S., 2021. Plastisphere in freshwaters: An emerging concern. Environ, Pollut. 290, 118123. https://doi.org/10.1016/ j.envpol.2021.118123.

Bastyans, S., Jackson, S., Fejer, G., 2022. Micro and nano-plastics, a threat to human health? Emerg. Top. Life Sci. 6, 411–422. https://doi.org/10.1042/ETLS20220024.

Bedrosian, N., Mitchell, E., Rohm, E., Rothe, M., Kelly, C., String, G., Lantagne, D., 2021. A systematic review of surface contamination, stability, and disinfection data on SARS- CoV-2 (Through july 10, 2020). Environ. Sci. Technol. 55, 4162–4173. https://doi.org/ 10.1021/acs.est.0c05651.

Belišová, N., Konečná, B., Bachratá, N., Ryba, J., Potočárová, A., Tamáš, M., Phuong, A.L., Púček, O., Kopáček, J., Mackul'ak, T.,

2022. Sorption of SARS-CoV-2 virus particles to the surface of microplastics released during washing processes. Int. J. Environ. Res. Public Health 19, 281. https://doi.org/10.3390/ijerph19010281.

Bennett-Lenane, H., Griffin, B.T., O'Shea, J.P., 2022. Machine learning methods for prediction of food effects on bioavailability: A comparison of support vector machines and artificial neural networks. Eur. J. Pharm. Sci. 168, 106018. https://doi.org/10.1016/j.ejps.2021.106018.

Bhagat, J., Nishimura, N., Shimada, Y., 2021. Toxicological interactions of microplastics/ nanoplastics and environmental contaminants: Current knowledge and future perspectives. J. Hazard. Mater. 405, 123913. https://doi.org/10.1016/j.jhazmat.2020.123913.

Bhaisare, M.L., Wu, B.-S., Wu, M.-C., Khan, M.S., Tseng, M.-H., Wu, H.-F., 2016. MALDI MS analysis, disk diffusion and optical density measurements for the antimicrobial effect of zinc oxide nanorods integrated in graphene oxide nanostructures. Biomater. Sci. 4, 183–194. https://doi.org/10.1039/c5bm00342c.

Bhatti, A., DeLong, R.K., 2023. Nanoscale interaction mechanisms of antiviral activity. ACS Pharmacol. Transl. Sci. 6, 220–228. https://doi.org/10.1021/acsptsci.2c00195.

Bhushan, M., Kumar, Y., Periyasamy, L., Viswanath, A.K., 2018. Antibacterial applications of α-Fe_2O_3/Co_3O_4 nanocomposites and study of their structural, optical, magnetic and cytotoxic characteristics. Appl. Nanosci. 8, 137–153. https://doi.org/10.1007/s13204-018-0656-5.

Bliss, C.I., 1939. The toxicity of poisons applied jointly. Ann. Appl. Biol. 26, 585–615. https://doi.org/10.1111/j.1744-7348.1939.tb06990.x.

Bopp, S.K., Barouki, R., Brack, W., Dalla Costa, S., Dorne, J.C.M., Drakvik, P.E., Faust, M., Karjalainen, T.K., Kephalopoulos, S., van Klaveren, J., Kolossa-Gehring, M., Kortenkamp, A., Lebret, E., Lettieri, T., Nørager, S., Rüegg, J., Tarazona, J.V., Trier, X., van de Water, B., van Gils, J., Bergman, Å., 2018. Current EU research activities on combined exposure to multiple chemicals. Environ. Int. 120, 544–562. https://doi.org/10.1016/j.envint.2018.07.037.

Böttcher, B., Nassal, M., 2018. Structure of mutant hepatitis B core protein capsids with premature secretion phenotype. J. Mol. Biol. 430, 4941–4954. https://doi.org/10.1016/j.jmb.2018.10.018.

Boughattas, I., Hattab, S., Zitouni, N., Mkhinini, M., Missawi, O., Bousserrhine, N., Banni, M., 2021. Assessing the presence of microplastic particles in tunisian agriculture soils and their potential toxicity effects using *Eisenia andrei* as bioindicator. Sci. Total Environ. 796, 148959. https://doi.org/10.1016/j.scitotenv.2021.148959.

Bouwmeester, H., Hollman, P.C.H., Peters, R.J.B., 2015. Potential health impact of environmentally released micro- and nanoplastics in the human food production chain: Experiences from nanotoxicology. Environ. Sci. Technol. 49, 8932–8947. https://doi.org/10.1021/acs.est.5b01090.

Braakhuis, H.M., Gosens, I., Heringa, M.B., Oomen, A.G., Vandebriel, R.J., Groenewold, M., Cassee, F.R., 2021. Mechanism of action of TiO_2: Recommendations to reduce uncertainties related to carcinogenic potential. Annu. Rev. Pharmacol. Toxicol. 61, 203–223. https://doi.org/10.1146/annurev-pharmtox-101419-100049.

Breisch, M., Loza, K., Pappert, K., Rostek, A., Rurainsky, C., Tschulik, K., Heggen, M., Epple, M., Tiller, J.C., Schildhauer, T.A., Köller, M., Sengstock, C., 2020. Enhanced dissolution of silver

nanoparticles in a physical mixture with platinum nanoparticles based on the sacrificial anode effect. Nanotechnology 31, 055703. https://doi.org/10.1088/1361-6528/ab4e48.

Brinkmann, B.W., Singhal, A., Sevink, G.J.A., Neeft, L., Vijver, M.G., Peijnenburg, W.J.G.M., 2022. Predicted adsorption affinity for enteric microbial metabolites to metal and carbon nanomaterials. J. Chem. Inf. Model. 62, 3589–3603. https://doi.org/10.1021/acs.jcim.2c00492.

Brisebois, E., Veillette, M., Dion-Dupont, V., Lavoie, J., Corbeil, J., Culley, A., Duchaine, C., 2018. Human viral pathogens are pervasive in wastewater treatment center aerosols. J. Environ. Sci. 67, 45–53. https://doi.org/10.1016/j.jes.2017.07.015.

Buglak, A.A., Zherdev, A.V., Dzantiev, B.B., 2019. Nano-(Q)SAR for cytotoxicity prediction of engineered nanomaterials. Molecules 24, 4537. https://doi.org/10.3390/molecules24244537.

Burley, S.K., Berman, H.M., Bhikadiya, C., Bi, C., Chen, L., Di Costanzo, L., Christie, C., Dalenberg, K., Duarte, J.M., Dutta, S., Feng, Z., Ghosh, S., Goodsell, D.S., Green, R.K., Guranović, V., Guzenko, D., Hudson, B.P., Kalro, T., Liang, Y., Lowe, R., Namkoong, H., Peisach, E., Periskova, I., Prlić, A., Randle, C., Rose, A., Rose, P., Sala, R., Sekharan, M., Shao, C., Tan, L., Tao, Y.-P., Valasatava, Y., Voigt, M., Westbrook, J., Woo, J., Yang, H., Young, J., Zhuravleva, M., Zardecki, C., 2019. RCSB protein data Bank: Biological macromolecular structures enabling research and education in fundamental biology, biomedicine, biotechnology and energy. Nucleic Acids Res. 47, D464–D474. https://doi.org/10.1093/nar/gky1004.

Buzea, C., Pacheco, I.I., Robbie, K., 2007. Nanomaterials and nanoparticles: Sources and toxicity. Biointerphases 2, MR17–MR172. https://doi.org/10.1116/1.2815690.

Campos, E.V.R., Pereira, A.E.S., Oliveira, J.L. de, Carvalho, L.B.,

Guilger-Casagrande, M., Lima, R. de, Fraceto, L.F., 2020. How can nanotechnology help to combat COVID-19? Opportunities and urgent need. J. Nanobiotechnol. 18, 125. https://doi.org/10.1186/s12951-020-00685-4.

Cao, J., Yang, Q., Jiang, J., Dalu, T., Kadushkin, A., Singh, J., Fakhrullin, R., Wang, F., Cai, X., Li, R., 2022. Coronas of micro/nano plastics: A key determinant in their risk assessments. Part. Fibre Toxicol. 19, 55. https://doi.org/10.1186/s12989-022-00492-9.

Casabianca, A., Orlandi, C., Amagliani, G., Magnani, M., Brandi, G., Schiavano, G.F., 2022. SARS-CoV-2 RNA detection on environmental surfaces in a university setting of Central Italy. Int. J. Environ. Res. Public Health 19, 5560. https://doi.org/10.3390/ijerph19095560.

Catarino, A.I., Macchia, V., Sanderson, W.G., Thompson, R.C., Henry, T.B., 2018. Low levels of microplastics (MP) in wild mussels indicate that MP ingestion by humans is minimal compared to exposure via household fibres fallout during a meal. Environ. Pollut. 237, 675–684. https://doi.org/10.1016/j.envpol.2018.02.069.

Chakraborty, D., Ethiraj, K.R., Chandrasekaran, N., Mukherjee, A., 2021. Mitigating the toxic effects of CdSe quantum dots towards freshwater alga *Scenedesmus obliquus*: Role of eco-corona. Environ. Pollut. 270, 116049. https://doi.org/10.1016/j.envpol.2020.116049.

Chao, S.-J., Huang, C.P., Lam, C.-C., Hua, L.-C., Chang, S.-H., Huang, C., 2021. Transformation of copper oxide nanoparticles as affected by ionic strength and its effects on the toxicity and bioaccumulation of copper in zebrafish embryo. Ecotoxicol. Environ. Saf. 225, 112759. https://doi.org/10.1016/j.ecoenv.2021.112759.

Chatterjee, M., Roy, K., 2023. "Data fusion" quantitative read-across structure-activity-activity relationships (q-RASAARs) for the prediction of toxicities of binary and ternary antibiotic mixtures toward three bacterial species. J. Hazard. Mater. 459, 132129. https://doi.org/10.1016/j.jhazmat.2023.132129.

Chen, G., Feng, Q., Wang, J., 2020. Mini-review of microplastics in the atmosphere and their risks to humans. Sci. Total Environ. 703, 135504. https://doi.org/10.1016/j.scitotenv.2019.135504.

Chen, G., Peijnenburg, W.J.G.M., Xiao, Y., Vijver, M.G., 2017. Current knowledge on the use of computational toxicology in hazard assessment of metallic engineered nanomaterials. Int. J. Mol. Sci. 18, 1504. https://doi.org/10.3390/ijms18071504.

Chen, G., Peijnenburg, W.J.G.M., Xiao, Y., Vijver, M.G., 2018. Developing species sensitivity distributions for metallic nanomaterials considering the characteristics of nanomaterials, experimental conditions, and different types of endpoints. Food Chem. Toxicol. 112, 563–570. https://doi.org/10.1016/j.fct.2017.04.003.

Chen, G., Vijver, M.G., Peijnenburg, W.J.G.M., 2015. Summary and analysis of the currently existing literature data on metal-based nanoparticles published for selected aquatic organisms: Applicability for toxicity prediction by (Q)SARs. Altern. Lab. Anim. 43, 221–240. https://doi.org/10.1177/026119291504300404.

Chen, L., Qian, Y., Jia, Q., Weng, R., Zhang, X., Li, Y., Qiu, J., 2023. A national-scale distribution of organochlorine pesticides (OCPs) in cropland soils and major types of food crops in China: Co-occurrence and associated risks. Sci. Total Environ. 861, 160637. https://doi.org/10.1016/j.scitotenv.2022.160637.

Chen, W., Duan, L., Zhu, D., 2007. Adsorption of polar and nonpolar organic chemicals to carbon nanotubes. Environ. Sci. Technol. 41,

8295–8300. https://doi.org/10.1021/es071230h.

Chen, X., Li, X., Li, Y., 2021. Toxicity inhibition strategy of microplastics to aquatic organisms through molecular docking, molecular dynamics simulation and molecular modification. Ecotoxicol. Environ. Saf. 226, 112870. https://doi.org/10.1016/j. ecoenv.2021.112870.

Chen, Y., Ma, J., Xu, M., Liu, S., 2020. Antiviral nanoagents: More attention and effort needed? Nano Today 35, 100976. https://doi.org/10.1016/j.nantod.2020.100976.

Chen, Y., Wang, M., Fu, H., Qu, X., Zhang, Z., Kang, F., Zhu, D., 2019. Spectroscopic and molecular modeling investigation on inhibition effect of nitroaromatic compounds on acetylcholinesterase activity. Chemosphere 236, 124365. https://doi.org/10.1016/j. chemosphere.2019.124365.

Chen, Z., Shi, X., Zhang, J., Wu, L., Wei, W., Ni, B.-J., 2023. Nanoplastics are significantly different from microplastics in urban waters. Water Res. X 19, 100169. https://doi.org/10.1016/j. wroa.2023.100169.

Cheng, C., Barceló, J., Hartnett, A.S., Kubinec, R., Messerschmidt, L., 2020. COVID-19 government response event dataset (CoronaNet v.1.0). Nat. Hum. Behav. 4, 756–768. https://doi.org/10.1038/ s41562-020-0909-7.

Conde-Cid, M., Arias-Estévez, M., Núñez-Delgado, A., 2021. SARS-CoV-2 and other pathogens could be determined in liquid samples from soils. Environ. Pollut. 273, 116445. https://doi.org/10.1016/ j.envpol.2021.116445.

Corpet, D.E., 2021. Why does SARS-CoV-2 survive longer on plastic than on paper? Med. Hypotheses 146, 110429. https://doi.org/ 10.1016/j.mehy.2020.110429.

Da Silva, G.H., Clemente, Z., Khan, L.U., Coa, F., Neto, L.L.R.,

Carvalho, H.W.P., Castro, V.L., Martinez, D.S.T., Monteiro, R.T.R., 2018. Toxicity assessment of TiO_2-MWCNT nanohybrid material with enhanced photocatalytic activity on *Danio rerio* (Zebrafish) embryos. Ecotoxicol. Environ. Saf. 165, 136–143. https://doi.org/10.1016/j.ecoenv.2018.08.093.

Das, J., Choi, Y.J., Song, H., Kim, J.H., 2016. Potential toxicity of engineered nanoparticles in mammalian germ cells and developing embryos: Treatment strategies and anticipated applications of nanoparticles in gene delivery. Hum. Reprod. Update 22, 588–619. https://doi.org/10.1093/humupd/dmw020.

Das, S., Thiagarajan, V., Chandrasekaran, N., Ravindran, B., Mukherjee, A., 2022. Nanoplastics enhance the toxic effects of titanium dioxide nanoparticle in freshwater algae *Scenedesmus obliquus*. Comp. Biochem. Phys. C 256, 109305. https://doi.org/10.1016/j.cbpc.2022.109305.

de Medeiros, A.M.Z., Khan, L.U., da Silva, G.H., Ospina, C.A., Alves, O.L., de Castro, V.L., Martinez, D.S.T., 2021. Graphene oxide-silver nanoparticle hybrid material: An integrated nanosafety study in zebrafish embryos. Ecotoxicol. Environ. Saf. 209, 111776. https://doi.org/10.1016/j.ecoenv.2020.111776.

de Souza Machado, A.A., Wood, C.M., Kloas, W., 2019. Novel concepts for novel entities: Updating ecotoxicology for a sustainable anthropocene. Environ. Sci. Technol. 53, 4680–4682. https://doi. org/10.1021/acs.est.9b02031.

Debeljak, P., Pinto, M., Proietti, M., Reisser, J., Ferrari, F.F., Abbas, B., van Loosdrecht, M.C.M., Slat, B., Herndl, G.J., 2017. Extracting DNA from ocean microplastics: A method comparison study. Anal. Methods 9, 1521–1526. https://doi.org/10.1039/C6AY03119F.

Demšar, J., Curk, T., Erjavec, A., Gorup, C., Hočevar, T., Milutinovič,

M., Možina, M., Polajnar, M., Toplak, M., Starič, A., Štajdohar, M., Umek, L., Žagar, L., Žbontar, J., Žitnik, M., Zupan, B., 2013. Orange: Data mining toolbox in python. J. Mach. Learn. Res. 14, 2349–2353.

Deng, R., Lin, D., Zhu, L., Majumdar, S., White, J.C., Gardea-Torresdey, J.L., Xing, B., 2017. Nanoparticle interactions with co-existing contaminants: Joint toxicity, bioaccumulation and risk. Nanotoxicology 11, 591–612. https://doi.org/10.1080/17435390.2017.1343404.

Deshwal, N., Singh, M.B., Bahadur, I., Kaushik, N., Kaushik, N.K., Singh, P., Kumari, K., 2023. A review on recent advancements on removal of harmful metal/metal ions using graphene oxide: Experimental and theoretical approaches. Sci. Total Environ. 858, 159672. https://doi.org/10.1016/j.scitotenv.2022.159672.

Diamond, M.L., de Wit, C.A., Molander, S., Scheringer, M., Backhaus, T., Lohmann, R., Arvidsson, R., Bergman, Å., Hauschild, M., Holoubek, I., Persson, L., Suzuki, N., Vighi, M., Zetzsch, C., 2015. Exploring the planetary boundary for chemical pollution. Environ. Int. 78, 8–15. https://doi.org/10.1016/j.envint.2015.02.001.

Diaz-Diestra, D.M., Palacios-Hernandez, T., Liu, Y., Smith, D.E., Nguyen, A.K., Todorov, T., Gray, P.J., Zheng, J., Skoog, S.A., Goering, P.L., 2022. Impact of surface chemistry of ultrasmall superparamagnetic iron oxide nanoparticles on protein corona formation and endothelial cell uptake, toxicity, and barrier function. Toxicol. Sci. 188, 261–275. https://doi.org/10.1093/toxsci/kfac058.

Diffenbaugh, N.S., Field, C.B., Appel, E.A., Azevedo, I.L., Baldocchi, D.D., Burke, M., Burney, J.A., Ciais, P., Davis, S.J., Fiore, A.M., Fletcher, S.M., Hertel, T.W., Horton, D.E., Hsiang, S.M., Jackson, R.B., Jin, X., Levi, M., Lobell, D.B., McKinley, G. A., Moore, F.C., Montgomery, A., Nadeau, K.C., Pataki, D.E.,

Randerson, J.T., Reichstein, M., Schnell, J.L., Seneviratne, S.I., Singh, D., Steiner, A.L., Wong-Parodi, G., 2020. The COVID-19 lockdowns: A window into the earth system. Nat. Rev. Earth Environ. 1, 470–481. https://doi.org/10.1038/s43017-020-0079-1.

Ding, L., Mao, R., Ma, S., Guo, X., Zhu, L., 2020. High temperature depended on the ageing mechanism of microplastics under different environmental conditions and its effect on the distribution of organic pollutants. Water Res. 174, 115634. https://doi.org/10.1016/j.watres.2020.115634.

Dong, X., Liu, X., Hou, Q., Wang, Z., 2023. From natural environment to animal tissues: A review of microplastics (nanoplastics) translocation and hazards studies. Sci. Total Environ. 855, 158686. https://doi.org/10.1016/j.scitotenv.2022.158686.

Dowlatabadi, M., Jahangiri, M., Farhadian, N., 2019. Prediction of chlortetracycline adsorption on the Fe_3O_4 nanoparticle using molecular dynamics simulation. J. Biomol. Struct. Dyn. 37, 3616–3626. https://doi.org/10.1080/07391102.2018.1521746.

Dris, R., Gasperi, J., Mirande, C., Mandin, C., Guerrouache, M., Langlois, V., Tassin, B., 2017. A first overview of textile fibers, including microplastics, in indoor and outdoor environments. Environ. Pollut. 221, 453–458. https://doi.org/10.1016/j.envpol.2016.12.013.

Dubey, A., Kotnala, G., Mandal, T.K., Sonkar, S.C., Singh, V.K., Guru, S.A., Bansal, A., Irungbam, M., Husain, F., Goswami, B., Kotnala, R.K., Saxena, S., Sharma, S.K., Saxena, K.N., Sharma, C., Kumar, S., Aswal, D.K., Manchanda, V., Koner, B.C., 2021. Evidence of the presence of SARS-CoV-2 virus in atmospheric air and surfaces of a dedicated COVID hospital. J. Med. Virol. 93, 5339–5349. https://doi.org/10.1002/jmv.27029.

Ehret, J., Vijver, M.G., Peijnenburg, W.J.G.M., 2014. The application of QSAR approaches to nanoparticles. Altern. Lab. Anim. 42, 43–50. https://doi.org/10.1177/026119291404200107.

Ekvall, M.T., Hedberg, J., Odnevall Wallinder, I., Malmendal, A., Hansson, L.-A., Cedervall, T., 2021. Adsorption of bio-organic eco-corona molecules reduces the toxic response to metallic nanoparticles in *Daphnia magna*. Sci. Rep. 11, 10784. https://doi.org/10.1038/s41598-021-90053-5.

Epa, V.C., Burden, F.R., Tassa, C., Weissleder, R., Shaw, S., Winkler, D.A., 2012. Modeling biological activities of nanoparticles. Nano Lett. 12, 5808–5812. https://doi.org/10.1021/nl303144k.

Feng, H., Liu, Y., Xu, Y., Li, S., Liu, X., Dai, Y., Zhao, J., Yue, T., 2022. Benzo[*a*]pyrene and heavy metal ion adsorption on nanoplastics regulated by humic acid: cooperation/competition mechanisms revealed by molecular dynamics simulations. J. Hazard. Mater. 424, 127431. https://doi.org/10.1016/j.jhazmat.2021.127431.

Feng, Y., Wu, J., Lu, H., Lao, W., Zhan, H., Lin, L., Liu, G., Deng, Y., 2023. Cytotoxicity and hemolysis of rare earth ions and nanoscale/bulk oxides (La, Gd, and Yb): Interaction with lipid membranes and protein corona formation. Sci. Total Environ. 879, 163259. https://doi.org/10.1016/j.scitotenv.2023.163259.

Fernandes, L.S., Galvão, A., Santos, R., Monteiro, S., 2023. Impact of water reuse on agricultural practices and human health. Environ. Res. 216, 114762. https://doi.org/10.1016/j.envres.2022.114762.

Florindo, H.F., Kleiner, R., Vaskovich-Koubi, D., Acúrcio, R.C., Carreira, B., Yeini, E., Tiram, G., Liubomirski, Y., Satchi-Fainaro, R., 2020. Immune-mediated approaches against COVID-19. Nat. Nanotechnol. 15, 630–645. https://doi.org/10.1038/s41565-020-0732-3.

Fournier, E., Etienne-Mesmin, L., Grootaert, C., Jelsbak, L., Syberg, K., Blanquet-Diot, S., Mercier-Bonin, M., 2021. Microplastics in

the human digestive environment: A focus on the potential and challenges facing *in vitro* gut model development. J. Hazard. Mater. 415, 125632. https://doi.org/10.1016/j.jhazmat.2021.125632.

Fred-Ahmadu, O.H., Bhagwat, G., Oluyoye, I., Benson, N.U., Ayejuyo, O.O., Palanisami, T., 2020. Interaction of chemical contaminants with microplastics: Principles and perspectives. Sci. Total Environ. 706, 135978. https://doi.org/10.1016/j.scitotenv.2019.135978.

Gajewicz, A., 2018. How to judge whether QSAR/read-across predictions can be trusted: A novel approach for establishing a model's applicability domain. Environ. Sci.: Nano 5, 408–421. https://doi.org/10.1039/C7EN00774D.

Gajewicz, A., Schaeublin, N., Rasulev, B., Hussain, S., Leszczynska, D., Puzyn, T., Leszczynski, J., 2015. Towards understanding mechanisms governing cytotoxicity of metal oxides nanoparticles: Hints from nano-QSAR studies. Nanotoxicology 9, 313–325. https://doi.org/10.3109/17435390.2014.930195.

Gastaldi, M.S., Felsztyna, I., Miguel, V., Sánchez-Borzone, M.E., García, D.A., 2023. Theoretical and experimental study of molecular interactions of fluralaner with lipid membranes. J. Agric. Food Chem. 71, 2134–2142. https://doi.org/10.1021/acs.jafc.2c06811.

Ge, C., Du, J., Zhao, L., Wang, L., Liu, Y., Li, D., Yang, Y., Zhou, R., Zhao, Y., Chai, Z., Chen, C., 2011. Binding of blood proteins to carbon nanotubes reduces cytotoxicity. Proc. Natl. Acad. Sci. 108, 16968–16973. https://doi.org/10.1073/pnas.1105270108.

Ge, L., Shao, B., Liang, Q., Huang, D., Liu, Z., He, Q., Wu, T., Luo, S., Pan, Y., Zhao, C., Huang, J., Hu, Y., 2022. Layered double hydroxide based materials applied in persulfate based advanced oxidation processes: Property, mechanism, application and

perspectives. J. Hazard. Mater. 424, 127612. https://doi.org/10.1016/j.jhazmat.2021.127612.

Geitner, N.K., Ogilvie Hendren, C., Cornelis, G., Kaegi, R., Lead, J.R., Lowry, G.V., Lynch, I., Nowack, B., Petersen, E., Bernhardt, E., Brown, S., Chen, W., de Garidel-Thoron, C., Hanson, J., Harper, S., Jones, K., von der Kammer, F., Kennedy, A., Kidd, J., Matson, C., Metcalfe, C.D., Pedersen, J., Peijnenburg, W.J.G.M., Quik, J.T.K., Rodrigues, S.M., Rose, J., Sayre, P., Simonin, M., Svendsen, C., Tanguay, R., Tefenkji, N., van Teunenbroek, T., Thies, G., Tian, Y., Rice, J., Turner, A., Liu, J., Unrine, J., Vance, M., White, J.C., Wiesner, M.R., 2020. Harmonizing across environmental nanomaterial testing media for increased comparability of nanomaterial datasets. Environ. Sci.: Nano 7, 13–36. https://doi.org/10.1039/c9en00448c.

Geitner, N.K., Zhao, W., Ding, F., Chen, W., Wiesner, M.R., 2017. Mechanistic insights from discrete molecular dynamics simulations of pesticide-nanoparticle interactions. Environ. Sci. Technol. 51, 8396–8404. https://doi.org/10.1021/acs.est.7b01674.

Georgantzopoulou, A., Farkas, J., Ndungu, K., Coutris, C., Carvalho, P.A., Booth, A.M., Macken, A., 2020. Wastewater-aged silver nanoparticles in single and combined exposures with titanium dioxide affect the early development of the marine copepod *Tisbe battagliai*. Environ. Sci. Technol. 54, 12316–12325. https://doi.org/10.1021/acs.est.0c03113.

Gidari, A., Sabbatini, S., Bastianelli, S., Pierucci, S., Busti, C., Bartolini, D., Stabile, A.M., Monari, C., Galli, F., Rende, M., Cruciani, G., Francisci, D., 2021. SARS-CoV-2 survival on surfaces and the effect of UV-C light. Viruses 13, 408. https://doi.org/10.3390/ v13030408.

Giner, B., Lafuente, C., Lapeña, D., Errazquin, D., Lomba, L., 2020. QSAR study for predicting the ecotoxicity of NADES towards

Aliivibrio fischeri. Exploring the use of mixing rules. Ecotoxicol. Environ. Saf. 191, 110004. https://doi.org/10.1016/j.ecoenv.2019.110004.

Gomes, S.I.L., Amorim, M.J.B., Pokhrel, S., Mädler, L., Fasano, M., Chiavazzo, E., Asinari, P., Jänes, J., Tämm, K., Burk, J., Scott-Fordsmand, J.J., 2021. Machine learning and materials modelling interpretation of *in Vivo* toxicological response to TiO_2 nano-particles library (UV and non-UV exposure). Nanoscale 13, 14666–14678. https://doi.org/10.1039/d1nr03231c.

Gonçalves, J., Koritnik, T., Mioč, V., Trkov, M., Bolješič, M., Berginc, N., Prosenc, K., Kotar, T., Paragi, M., 2021. Detection of SARS-CoV-2 RNA in hospital wastewater from a low COVID-19 disease prevalence area. Sci. Total Environ. 755, 143226. https://doi. org/10.1016/j.scitotenv.2020.143226.

Gong, H., Li, R., Li, F., Guo, X., Xu, L., Gan, L., Yan, M., Wang, J., 2023. Toxicity of nanoplastics to aquatic organisms: Genotoxicity, cytotoxicity, individual level and beyond individual level. J. Hazard. Mater. 443, 130266. https://doi.org/10.1016/j.jhazmat.2022.130266.

González-Pleiter, M., Edo, C., Aguilera, Á., Viúdez-Moreiras, D., Pulido-Reyes, G., González-Toril, E., Osuna, S., de Diego-Castilla, G., Leganés, F., Fernández-Piñas, F., Rosal, R., 2021. Occurrence and transport of microplastics sampled within and above the planetary boundary layer. Sci. Total Environ. 761, 143213. https://doi.org/10.1016/j.scitotenv.2020.143213.

Guineé, J.B., Heijungs, R., Vijver, M.G., Peijnenburg, W.J.G.M., 2017. Setting the stage for debating the roles of risk assessment and life-cycle assessment of engineered nanomaterials. Nat. Nanotechnol. 12, 727–733. https://doi.org/10.1038/nnano.2017.135.

Gunathilake, T.M.S.U., Ching, Y.C., Uyama, H., Hai, N.D., Chuah,

C.H., 2022. Enhanced curcumin loaded nanocellulose: A possible inhalable nanotherapeutic to treat COVID-19. Cellulose 29, 1821–1840. https://doi.org/10.1007/s10570-021-04391-8.

Guo, X., Liu, Y., Wang, J., 2019. Sorption of sulfamethazine onto different types of microplastics: A combined experimental and molecular dynamics simulation study. Mar. Pollut. Bull. 145, 547–554. https://doi.org/10.1016/j.marpolbul.2019.06.063.

Haghighat, F., Kim, Y., Sourinejad, I., Yu, I.J., Johari, S.A., 2021. Titanium dioxide nanoparticles affect the toxicity of silver nanoparticles in common carp (*Cyprinus carpio*). Chemosphere 262, 127805. https://doi.org/10.1016/j.chemosphere.2020.127805.

Han, J., Zhang, X., He, S., Jia, P., 2021. Can the coronavirus disease be transmitted from food? A review of evidence, risks, policies and knowledge gaps. Environ. Chem. Lett. 19, 5–16. https://doi.org/10.1007/s10311-020-01101-x.

Haynes, W.M., 2011. CRC Handbook of Chemistry and Physics, 92nd Edition, CRC Press.

He, M., Liang, Q., Tang, L., Liu, Z., Shao, B., He, Q., Wu, T., Luo, S., Pan, Y., Zhao, C., Niu, C., Hu, Y., 2021. Advances of covalent organic frameworks based on magnetism: Classification, synthesis, properties, applications. Coord. Chem. Rev. 449, 214219. https://doi.org/10.1016/j.ccr.2021.214219.

Hernández-Moreno, D., Valdehita, A., Conde, E., Rucandio, I., Navas, J.M., Fernández-Cruz, M.L., 2019. Acute toxic effects caused by the co-exposure of nanoparticles of ZnO and Cu in rainbow trout. Sci. Total Environ. 687, 24–33. https://doi.org/10.1016/j.scitotenv.2019.06.084.

Hong, H., Adam, V., Nowack, B., 2021. Form-specific and probabilistic environmental risk assessment of 3 engineered nanomaterials (nano-Ag, nano-TiO_2, and nano-ZnO) in European

freshwaters. Environ. Toxicol. Chem. 40, 2629–2639. https://doi.org/10. 1002/etc.5146.

Huang, Q., Yu, L., Petros, A.M., Gunasekera, A., Liu, Z., Xu, N., Hajduk, P., Mack, J., Fesik, S.W., Olejniczak, E.T., 2004. Structure of the N-terminal RNA-binding domain of the SARS CoV nucleocapsid protein. Biochemistry 43, 6059–6063. https://doi. org/10.1021/bi036155b.

Huang, Y., Li, X., Xu, S., Zheng, H., Zhang, L., Chen, J., Hong, H., Kusko, R., Li, R., 2020. Quantitative structure-activity relationship models for predicting inflammatory potential of metal oxide nanoparticles. Environ. Health Perspect. 128, 67010. https://doi.org/10.1289/EHP6508.

Hutchison, J.E., 2016. The road to sustainable nanotechnology: Challenges, progress and opportunities. ACS Sustainable Chem. Eng. 4, 5907–5914. https://doi.org/10.1021/acssuschemeng. 6b02121.

Innocenzi, P., Stagi, L., 2020. Carbon-based antiviral nanomaterials: Graphene, C-dots, and fullerenes. A perspective. Chem. Sci. 11, 6606–6622. https://doi.org/10.1039/D0SC02658A.

Jahan, S., Alias, Y.B., Bakar, A.F.B.A., Yusoff, I.B., 2018. Toxicity evaluation of ZnO and TiO_2 nanomaterials in hydroponic red bean (*Vigna angularis*) plant: Physiology, biochemistry and kinetic transport. J. Environ. Sci. 72, 140–152. https://doi.org/ 10.1016/j.jes.2017.12.022.

Jaworska, J., Nikolova-Jeliazkova, N., Aldenberg, T., 2005. QSAR applicabilty domain estimation by projection of the training set descriptor space: A review. Altern. Lab. Anim. 33, 445–459. https://doi.org/10.1177/026119290503300508.

Jayaramulu, K., Mukherjee, S., Morales, D.M., Dubal, D.P., Nanjundan, A.K., Schneemann, A., Masa, J., Kment, S., Schuhmann, W., Otyepka, M., Zbořil, R., Fischer, R.A., 2022.

Graphene-based metal–organic framework hybrids for applications in catalysis, environmental, and energy technologies. Chem. Rev. 122, 17241–17338. https://doi.org/10.1021/acs.chemrev.2c00270.

Jennings, W.G., Perez, N.M., 2020. The immediate impact of COVID-19 on law enforcement in the United States. Am. J. Crim. Justice 45, 690–701. https://doi.org/10.1007/s12103-020-09536-2.

Ji, L., Chen, W., Xu, Z., Zheng, S., Zhu, D., 2013. Graphene nanosheets and graphite oxide as promising adsorbents for removal of organic contaminants from aqueous solution. J. Environ. Qual. 42, 191–198. https://doi.org/10.2134/jeq2012.0172.

Ji, Z., Guo, W., Wood, E.L., Liu, J., Sakkiah, S., Xu, X., Patterson, T.A., Hong, H., 2022. Machine learning models for predicting cytotoxicity of nanomaterials. Chem. Res. Toxicol. 35, 125–139. https://doi.org/10.1021/acs.chemrestox.1c00310.

Jia, Y., Hou, X., Wang, Z., Hu, X., 2021. Machine learning boosts the design and discovery of nanomaterials. ACS Sustainable Chem. Eng. 9, 6130–6147. https://doi.org/10.1021/acssuschemeng.1c00483.

Jogaiah, S., Paidi, M.K., Venugopal, K., Geetha, N., Mujtaba, M., Udikeri, S.S., Govarthanan, M., 2021. Phytotoxicological effects of engineered nanoparticles: An emerging nanotoxicology. Sci. Total Environ. 801, 149809. https://doi.org/10.1016/j.scitotenv.2021.149809.

Jośko, I., Krasucka, P., Skwarek, E., Oleszczuk, P., Sheteiwy, M., 2022. The co-occurrence of Zn-and Cu-based engineered nanoparticles in soils: The metal extractability vs. toxicity to *Folsomia candida*. Chemosphere 287, 132252. https://doi.org/10.1016/j. chemosphere.2021.132252.

Jośko, I., Kusiak, M., Xing, B., Oleszczuk, P., 2021. Combined effect of nano-CuO and nano-ZnO in plant-related system: From bioavailability in soil to transcriptional regulation of metal homeostasis in barley. J. Hazard. Mater. 416, 126230. https://doi.org/10.1016/j.jhazmat.2021.126230.

Junaid, M., Liu, S., Chen, G., Liao, H., Wang, J., 2023. Transgenerational impacts of micro(nano)plastics in the aquatic and terrestrial environment. J. Hazard. Mater. 443, 130274. https://doi.org/10.1016/j.jhazmat.2022.130274.

Junaid, M., Liu., S, Liao, H., Liu, X., Wu, Y., Wang, J., 2022. Wastewater plastisphere enhances antibiotic resistant elements, bacterial pathogens, and toxicological impacts in the environment. Sci. Total Environ. 841, 156805. https://doi.org/ 10.1016/j. scitotenv.2022.156805.

Junaid, M., Wang, J., 2022. Interaction of micro(nano)plastics with extracellular and intracellular biomolecules in the freshwater environment. Crit. Rev. Env. Sci. Tec. 52, 4241–4265. https://doi.org/10.1080/10643389.2021.2002078.

Jung, Y.S., Sampath, V., Prunicki, M., Aguilera, J., Allen, H., LaBeaud, D., Veidis, E., Barry, M., Erny, B., Patel, L., Akdis, C., Akdis, M., Nadeau, K., 2022. Characterization and regulation of microplastic pollution for protecting planetary and human health. Environ. Pollut. 315, 120442. https://doi.org/10.1016/j.envpol. 2022.120442.

Kang, S., Yang, M., Hong, Z., Zhang, L., Huang, Z., Chen, X., He, S., Zhou, Z., Zhou, Z., Chen, Q., Yan, Y., Zhang, C., Shan, H., Chen, S., 2020. Crystal structure of SARS-CoV-2 nucleocapsid protein RNA binding domain reveals potential unique drug targeting sites. Acta Pharm. Sin. B 10, 1228–1238. https://doi.org/10. 1016/j.apsb. 2020.04.009.

Kar, S., Gajewicz, A., Puzyn, T., Roy, K., Leszczynski, J., 2014.

Periodic table-based descriptors to encode cytotoxicity profile of metal oxide nanoparticles: A mechanistic QSTR approach. Ecotoxicol. Environ. Saf. 107, 162–169. https://doi.org/10.1016/j.ecoenv. 2014.05.026.

Kar, S., Leszczynski, J., 2019. Exploration of computational approaches to predict the toxicity of chemical mixtures. Toxics 7, 15. https://doi.org/10.3390/toxics7010015.

Kar, S., Pathakoti, K., Leszczynska, D., Tchounwou, P.B., Leszczynski, J., 2022. *In vitro* and *in silico* study of mixtures cytotoxicity of metal oxide nanoparticles to *Escherichia coli*: A mechanistic approach. Nanotoxicology 16, 566–579. https://doi.org/10.1080/17435390.2022.2123750.

Katsumiti, A., Losada-Carrillo, M.P., Barros, M., Cajaraville, M.P., 2021. Polystyrene nanoplastics and microplastics can act as Trojan horse carriers of benzo(*a*)pyrene to mussel hemocytes in vitro. Sci. Rep. 11, 22396. https://doi.org/10.1038/s41598-021-01938-4.

Kaul, S., Gulati, N., Verma, D., Mukherjee, S., Nagaich, U., 2018. Role of nanotechnology in cosmeceuticals: A review of recent advances. J. Pharm. 2018, 3420204. https://doi.org/10.1155/2018/3420204.

Kaur, J., Khatri, M., Puri, S., 2019. Toxicological evaluation of metal oxide nanoparticles and mixed exposures at low doses using zebra fish and THP1 cell line. Environ. Toxicol. 34, 375–387. https://doi.org/10.1002/tox.22692.

Khoo, K.S., Ho, L.Y., Lim, H.R., Leong, H.Y., Chew, K.W., 2021. Plastic waste associated with the COVID-19 pandemic: Crisis or opportunity? J. Hazard. Mater. 417, 126108. https://doi.org/10.1016/j.jhazmat.2021.126108.

Kim, D., Chae, Y., An, Y.-J., 2017. Mixture toxicity of nickel and microplastics with different functional groups on *Daphnia*

magna. Environ. Sci. Technol. 51, 12852–12858. https://doi.org/10.1021/acs.est.7b03732.

Kim, J.-M., Chung, Y.-S., Jo, H.J., Lee, N.-J., Kim, M.S., Woo, S.H., Park, S., Kim, J.W., Kim, H.M., Han, M.-G., 2020. Identification of coronavirus isolated from a patient in Korea with COVID-19. Osong Public Health Res. Perspect. 11, 3–7. https://doi.org/10.24171/j.phrp.2020.11.1.02.

Kim, L., Cui, R., Il Kwak, J., An, Y.-J., 2022. Trophic transfer of nanoplastics through a microalgae-crustacean-small yellow croaker food chain: Inhibition of digestive enzyme activity in fish. J. Hazard. Mater. 440, 129715. https://doi.org/10.1016/j.jhazmat.2022.129715.

Kitajima, M., Ahmed, W., Bibby, K., Carducci, A., Gerba, C.P., Hamilton, K.A., Haramoto, E., Rose, J.B., 2020. SARS-CoV-2 in wastewater: State of the knowledge and research needs. Sci. Total Environ. 739, 139076. https://doi.org/10.1016/j.scitotenv.2020.139076.

Kolarević, S., Micsinai, A., Szántó-Egész, R., Lukács, A., Kračun-Kolarević, M., Djordjevic, A., Vojnović-Milutinović, D., Marić, J.J., Kirschner, A.K.T., Farnleitner, A.A.H., Linke, R., Đukic, A., Kostić-Vuković, J., Paunović, M., 2022. Wastewater-based epidemiology in countries with poor wastewater treatment – Epidemiological indicator function of SARS-CoV-2 RNA in surface waters. Sci. Total Environ. 843, 156964. https://doi.org/10.1016/j.scitotenv.2022.156964.

Koppenol, W.H., 2001. "The Haber-Weiss cycle-70 years later." REDOX Report: Communications in Free Radical Research 6, 229–234. https://doi.org/10.1179/135100001101536373.

Kostarelos, K., 2020. Nanoscale nights of COVID-19. Nat. Nanotechnol. 15, 343–344. https://doi.org/10.1038/s41565-020-0687-4.

Kubinyi, H., 1993. QSAR: Hansch analysis and related approaches, in: Mann-hold, R., Krogsgaard-Larsen, P., Timmerman, H. (Eds.), Methods and principles in medicinal chemistry, vol 1. VCH, Weinheim. https://doi.org/10.1002/9783527616824.

Kumar, M., Patel, A.K., Shah, A.V., Raval, J., Rajpara, N., Joshi, M., Joshi, C.G., 2020. First proof of the capability of wastewater surveillance for COVID-19 in India through detection of genetic material of SARS-CoV-2. Sci. Total Environ. 746, 141326. https://doi.org/10.1016/j.scitotenv.2020.141326.

Kumar, N., Shah, V., Walker, V.K., 2012. Influence of a nanoparticle mixture on an arctic soil community. Environ. Toxicol. Chem. 31, 131–135. https://doi.org/10.1002/etc.721.

Kumar, P., Mahajan, P., Kaur, R., Gautam, S., 2020. Nanotechnology and its challenges in the food sector: A review. Mater. Today Chem. 17, 100332. https://doi.org/10.1016/j.mtchem.2020.100332.

Kuznetsova, O.V., Keppler, B.K., Timerbaev, A.R., 2023. Analysis of engineered nanoparticles in seawater using ICP-MS-based technology: From negative to positive samples. Molecules 28, 994. https://doi.org/10.3390/molecules28030994.

La Rosa, G., Iaconelli, M., Mancini, P., Bonanno Ferraro, G., Veneri, C., Bonadonna, L., Lucentini, L., Suffredini, E., 2020. First detection of SARS-CoV-2 in untreated wastewaters in Italy. Sci. Total Environ. 736, 139652. https://doi.org/10.1016/j.scitotenv.2020.139652.

Lai, R.W.S., Zhou, G.-J., Kang, H.-M., Jeong, C.-B., Djurišić, A.B., Lee, J.-S., Leung, K.M.Y., 2022. Contrasting toxicity of polystyrene nanoplastics to the rotifer *Brachionus koreanus* in the presence of zinc oxide nanoparticles and zinc ions. Aquat. Toxicol. 253, 106332. https://doi.org/10.1016/j.aquatox.2022.106332.

Lamers, M.M., Beumer, J., van der Vaart, J., Knoops, K., Puschhof, J.,

Breugem, T.I., Ravelli, R.B.G., Paul van Schayck, J., Mykytyn, A.Z., Duimel, H.Q., van Donselaar, E., Riesebosch, S., Kuijpers, H.J.H., Schipper, D., van de Wetering, W.J., de Graaf, M., Koopmans, M., Cuppen, E., Peters, P.J., Haagmans, B.L., Clevers, H., 2020. SARS-CoV-2 productively infects human gut enterocytes. Science 369, 50–54. https://doi.org/10.1126/science.abc1669.

Lan, T.C.T., Allan, M.F., Malsick, L.E., Woo, J.Z., Zhu, C., Zhang, F., Khandwala, S., Nyeo, S.S.Y., Sun, Y., Guo, J.U., Bathe, M., Näär, A., Griffiths, A., Rouskin, S., 2022. Secondary structural ensembles of the SARS-CoV-2 RNA genome in infected cells. Nat. Commun. 13, 1128. https://doi.org/10.1038/s41467-022-28603-2.

Langeveld, J., Schilperoort, R., Heijnen, L., Elsinga, G., Schapendonk, C.E.M., Fanoy, E., de Schepper, E.I.T., Koopmans, M.P.G., de Graaf, M., Medema, G., 2023. Normalisation of SARS-CoV-2 concentrations in wastewater: The use of flow, electrical conductivity and crAssphage. Sci. Total Environ. 865, 161196. https://doi.org/10.1016/j.scitotenv.2022.161196.

LeBlanc, R.M., Kasprzak, W.K., Longhini, A.P., Olenginski, L.T., Abulwerdi, F., Ginocchio, S., Shields, B., Nyman, J., Svirydava, M., Del Vecchio, C., Ivanic, J., Schneekloth Jr., J.S., Shapiro, B.A., Dayie, T.K., Le Grice, S.F.J., 2022. Structural insights of the conserved "priming loop" of hepatitis B virus pre-genomic RNA. J. Biomol. Struct. Dyn. 40, 9761–9773. https://doi.org/10.1080/07391102.2021.1934544.

Lee, H., Ju, M., Kim, Y., 2020. Estimation of emission of tire wear particles (TWPs) in Korea. Waste Manag. 108, 154–159. https://doi.org/10.1016/j.wasman.2020.04.037.

Lee, H., Shim, W.J., Kwon, J.-H., 2014. Sorption capacity of plastic debris for hydrophobic organic chemicals. Sci. Total Environ. 470–471, 1545–1552. https://doi.org/10.1016/j.scitotenv.2013.

08.023.

Lee, M., Kim, H., Ryu, H.-S., Moon, J., Khant, N.A., Yu, C., Yu, J.-H., 2022. Review on invasion of microplastic in our ecosystem and implications. Sci. Prog. 105. https://doi.org/10.1177/00368504221140766.

Leonel, A.G., Mansur, A.A.P., Mansur, H.S., 2021. Advanced functional nanostructures based on magnetic iron oxide nanomaterials for water remediation: A review. Water Res. 190, 116693. https://doi.org/10.1016/j.watres.2020.116693.

Li, M., Liu, W., Slaveykova, V.I., 2020. Effects of mixtures of engineered nanoparticles and metallic pollutants on aquatic organisms. Environments 7, 27. https://doi.org/10.3390/environments7040027.

Li, R., Zhu, L., Yang, K., Li, H., Zhu, Y.-G., Cui, L., 2021. Impact of urbanization on anti- biotic resistome in different microplastics: Evidence from a large-scale whole river analysis. Environ. Sci. Technol. 55, 8760–8770. https://doi.org/10.1021/acs.est.1c01395.

Li, S., Liu, X., Liu, G., Liu, C., 2023. Biomimetic nanotechnology for SARS-CoV-2 treatment. Viruses 15, 596. https://doi.org/10.3390/v15030596.

Li, X., Yang, B., Yang, J., Fan, Y., Qian, X., Li, H., 2021. Magnetic properties and its application in the prediction of potentially toxic elements in aquatic products by machine learning. Sci. Total Environ. 783, 147083. https://doi.org/10.1016/j.scitotenv.2021.147083.

Liang, Q., Shao, B., Tong, S., Liu, Z., Tang, L., Liu, Y., Cheng, M., He, Q., Wu, T., Pan, Y., Huang, J., Peng, Z., 2021. Recent advances of melamine self-assembled graphitic carbon nitride-based materials: Design, synthesis and application in energy and environment. Chem. Eng. J. 405, 126951. https://doi.org/

10.1016/j.cej.2020.126951.

Liu, N., Liang, Y., Wei, T., Zou, L., Bai, C., Huang, X., Wu, T., Xue, Y., Tang, M., Zhang, T., 2022. Protein corona mitigated the cytotoxicity of CdTe QDs to macrophages by targeting mitochondria. NanoImpact 25, 100367. https://doi.org/10.1016/j.impact.2021.100367.

Liu, P., Yang, M., Zhao, X., Guo, Y., Wang, L., Zhang, J., Lei, W., Han, W., Jiang, F., Liu, W.J., Gao, G.F., Wu, G., 2020. Cold-chain transportation in the frozen food industry may have caused a recurrence of COVID-19 cases in destination: Successful isolation of SARS-CoV-2 virus from the imported frozen cod package surface. Biosaf. Health 2, 199–201. https://doi.org/10.1016/j.bsheal.2020.11.003.

Liu, Q., Schauer, J., 2021. Airborne microplastics from waste as a transmission vector for COVID-19. Aerosol Air Qual. Res. 21, 200439. https://doi.org/10.4209/aaqr.2020.07.0439.

Liu, R., Zhang, H.Y., Ji, Z.X., Rallo, R., Xia, T., Chang, C.H., Nel, A., Cohen, Y., 2013. Development of structure–activity relationship for metal oxide nanoparticles. Nanoscale 5, 5644–5653. https://doi.org/10.1039/c3nr01533e.

Liu, S., Zhang, X., Zeng, K., He, C., Huang, Y., Xin, G., Huang, X., 2023. Insights into eco-corona formation and its role in the biological effects of nanomaterials from a molecular mechanisms perspective. Sci. Total Environ. 858, 159867. https://doi.org/10.1016/j.scitotenv.2022.159867.

Liu, Y., Baas, J., Peijnenburg, W.J.G.M., Vijver, M.G., 2016. Evaluating the combined toxicity of Cu and ZnO nanoparticles: Utility of the concept of additivity and a nested experimental design. Environ. Sci. Technol. 50, 5328–5337. https://doi.org/10.1021/acs.est. 6b00614.

Liu, Yanjun, Huang, Z., Zhou, J., Tang, J., Yang, C., Chen, C., Huang,

W., Dang, Z., 2020. Influence of environmental and biological macromolecules on aggregation kinetics of nanoplastics in aquatic systems. Water Res. 186, 116316. https://doi.org/10.1016/j.watres.2020.116316.

Liu, Y., Vijver, M.G., Pan, B., Peijnenburg, W.J.G.M., 2017. Toxicity models of metal mixtures established on the basis of "additivity" and "interactions". Front. Environ. Sci. Eng. 11, 10–13. https://doi.org/10.1007/s11783-017-0916-8.

Liu, Yuan, Ning, Z., Chen, Y., Guo, M., Liu, Y., Gali, N.K., Sun, L., Duan, Y., Cai, J., Westerdahl, D., Liu, X., Xu, K., Ho, K.-F., Kan, H., Fu, Q., Lan, K., 2020. Aerodynamic analysis of SARS-CoV-2 in two Wuhan hospitals. Nature 582, 557–560. https://doi.org/10.1038/s41586-020-2271-3.

Łoczechin, A., Séron, K., Barras, A., Giovanelli, E., Belouzard, S., Chen, Y.-T., Metzler-Nolte, N., Boukherroub, R., Dubuisson, J., Szunerits, S., 2019. Functional carbon quantum dots as medical countermeasures to human coronavirus. ACS Appl. Mater. Interfaces 11, 42964–42974. https://doi.org/10.1021/acsami.9b15032.

Loewe, S., Muischneck, H., 1926. Effect of combinations: Mathematical basis of problem. Arch. Exp. Pathol. Pharmakol. 114, 313–326.

Londono, N., Donovan, A.R., Shi, H., Geisler, M., Liang, Y., 2019. Effects of environmentally relevant concentrations of mixtures of TiO_2, ZnO and Ag ENPs on a river bacterial community. Chemosphere 230, 567–577. https://doi.org/10.1016/j.chemosphere.2019.05.110.

Lopes, S., Pinheiro, C., Soares, A.M.V.M., Loureiro, S., 2016. Joint toxicity prediction of nanoparticles and ionic counterparts: Simulating toxicity under a fate scenario. J. Hazard. Mater. 320, 1–9. https://doi.org/10.1016/j.jhazmat.2016.07.068.

Lowry, G.V., Avellan, A., Gilbertson, L.M., 2019. Opportunities and challenges for nanotechnology in the agri-tech revolution. Nat. Nanotechnol. 14, 517–522. https://doi.org/10.1038/s41565-019-0461-7.

Lowry, G.V., Gregory, K.B., Apte, S.C., Lead, J.R., 2012. Transformations of nanomaterials in the environment. Environ. Sci. Technol. 46, 6893–6899. https://doi.org/10.1021/es300839e.

Lu, J., Yu, Z., Ngiam, L., Guo, J., 2022. Microplastics as potential carriers of viruses could prolong virus survival and infectivity. Water Res. 225, 119115. https://doi.org/10.1016/j.watres.2022.119115.

Lu, T., Chen, F., 2012a. Multiwfn: A multifunctional wavefunction analyzer. J. Comput. Chem. 33, 580–592. https://doi.org/10.1002/jcc.22885.

Lu, T., Chen, F., 2012b. Quantitative analysis of molecular surface based on improved Marching Tetrahedra algorithm. J. Mol. Graph. Model. 38, 314–323. https://doi.org/10.1016/j.jmgm.2012.07.004.

Luo, H., Du, Q., Zhong, Z., Xu, Y., Peng, J., 2022. Protein-coated microplastics corona complex: An underestimated risk of microplastics. Sci. Total Environ. 851, 157948. https://doi.org/10.1016/j.scitotenv.2022.157948.

Ma, J., Chen, F., Xu, H., Jiang, H., Liu, J., Li, P., Chen, C.C., Pan, K., 2021. Face masks as a source of nanoplastics and microplastics in the environment: Quantification, characterization, and potential for bioaccumulation. Environ. Pollut. 288, 117748. https://doi. org/10.1016/j.envpol.2021.117748.

MacLeod, M., Breitholtz, M., Cousins, I.T., de Wit, C.A., Persson, L.M., Rudén, C., McLachlan, M.S., 2014. Identifying chemicals that are planetary boundary threats. Environ. Sci. Technol. 48, 11057–

11063. https://doi.org/10.1021/es501893m.

Maestre, J.P., Jarma, D., Yu, J.-R.F., Siegel, J.A., Horner, S.D., Kinney, K.A., 2021. Distribution of SARS-CoV-2 RNA signal in a home with COVID-19 positive occupants. Sci. Total Environ. 778, 146201. https://doi.org/10.1016/j.scitotenv.2021.146201.

Maleki Dizaj, S., Mennati, A., Jafari, S., Khezri, K., Adibkia, K., 2015. Antimicrobial activity of carbon-based nanoparticles. Adv. Pharm. Bull. 5, 19–23. https://doi.org/10.5681/apb.2015.003.

Mansouri, B., Maleki, A., Johari, S.A., Shahmoradi, B., Mohammadi, E., Shahsavari, S., Davari, B., 2016. Copper bioaccumulation and depuration in common carp (*Cyprinus carpio*) following co-exposure to TiO_2 and CuO nanoparticles. Arch. Environ. Contam. Toxicol. 71, 541–552. https://doi.org/10.1007/s00244-016-0313-5.

Martín-de-Lucía, I., Gonçalves, S.F., Leganés, F., Fernández-Piñas, F., Rosal, R., Loureiro, S., 2019. Combined toxicity of graphite-diamond nanoparticles and thiabendazole to *Daphnia magna*. Sci. Total Environ. 688, 1145–1154. https://doi.org/10.1016/j.scitotenv.2019.06.316.

Martinez, D.S.T., Ellis, L.-J.A., Da Silva, G.H., Petry, R., Medeiros, A.M.Z., Davoudi, H.H., Papadiamantis, A.G., Fazzio, A., Afantitis, A., Melagraki, G., Lynch, I., 2022. *Daphnia magna* and mixture toxicity with nanomaterials–current status and perspectives in data-driven risk prediction. Nano Today 43, 101430. https://doi. org/10.1016/j.nantod.2022.101430.

Matson, M.J., Yinda, C.K., Seifert, S.N., Bushmaker, T., Fischer, R.J., van Doremalen, N., Lloyd-Smith, J.O., Munster, V.J., 2020. Effect of environmental conditions on SARS-CoV-2 stability in human nasal mucus and sputum. Emerg. Infect. Dis. 26, 2276–2278. https://doi.org/10.3201/eid2609.202267.

Mei, M., Tan, X., 2021. Current strategies of antiviral drug discovery

for COVID-19. Front. Mol. Biosci. 8, 671263. https://doi.org/10.3389/fmolb.2021.671263.

Menéndez-Pedriza, A., Jaumot, J., 2020. Interaction of environmental pollutants with microplastics: A critical review of sorption factors, bioaccumulation and ecotoxicological effects. Toxics 8, 40. https://doi.org/10.3390/toxics8020040.

Meo, S.A., Almutairi, F.J., Abukhalaf, A.A., Alessa, O.M., Al-Khlaiwi, T., Meo, A.S., 2021. Sandstorm and its effect on particulate matter PM 2.5, carbon monoxide, nitrogen dioxide, ozone pollutants and SARS-CoV-2 cases and deaths. Sci. Total Environ. 795, 148764. https://doi.org/10.1016/j.scitotenv.2021.148764.

Mercogliano, R., Avio, C.G., Regoli, F., Anastasio, A., Colavita, G., Santonicola, S., 2020. Occurrence of microplastics in commercial seafood under the perspective of the human food chain. A review. J. Agric. Food Chem. 68, 5296–5301. https://doi.org/10.1021/acs.jafc.0c01209.

Mikolajczyk, A., Gajewicz, A., Mulkiewicz, E., Rasulev, B., Marchelek, M., Diak, M., Hirano, S., Zaleska-Medynska, A., Puzyn, T., 2018. Nano-QSAR modeling for ecosafe design of heterogeneous TiO_2-based nano-photocatalysts. Environ. Sci.: Nano 5, 1150–1160. https://doi.org/10.1039/C8EN00085A.

Mikolajczyk, A., Malankowska, A., Nowaczyk, G., Gajewicz, A., Hirano, S., Jurga, S., Zaleska-Medynska, A., Puzyn, T., 2016. Combined experimental and computational approach to developing efficient photocatalysts based on Au/Pd–TiO_2 nanoparticles. Environ. Sci.: Nano, 3, 1425–1435. https://doi.org/10.1039/c6en00232c.

Mikolajczyk, A., Sizochenko, N., Mulkiewicz, E., Malankowska, A., Rasulev, B., Puzyn, T., 2019. A chemoinformatics approach for the characterization of hybrid nanomaterials: Safer and efficient design perspective. Nanoscale 11, 11808–11818. https://doi.org/

10.1039/c9nr01162e.

Minetto, D., Volpi, Ghirardini A., Libralato, G., 2016. Saltwater ecotoxicology of Ag, Au, CuO, TiO_2, ZnO and C_{60} engineered nanoparticles: An overview. Environ. Int. 92–93, 189–201. https://doi.org/10.1016/j.envint.2016.03.041.

Mohan, S.V., Hemalatha, M., Kopperi, H., Ranjith, I., Kumar, A.K., 2021. SARS-CoV-2 in environmental perspective: Occurrence, persistence, surveillance, inactivation and challenges. Chem. Eng. J. 405, 126893. https://doi.org/10.1016/j.cej.2020.126893.

Morawska, L., Cao, J., 2020. Airborne transmission of SARS-CoV-2: The world should face the reality. Environ. Int. 139, 105730. https://doi.org/10.1016/j.envint.2020.105730.

Moreno, T., Pintó, R.M., Bosch, A., Moreno, N., Alastuey, A., Minguillón, M.C., Anfruns-Estrada, E., Guix, S., Fuentes, C., Buonanno, G., Stabile, L., Morawska, L., Querol, X., 2021. Tracing surface and airborne SARS-CoV-2 RNA inside public buses and subway trains. Environ. Int. 147, 106326. https://doi.org/10. 1016/j.envint.2020.106326.

Moresco, V., Oliver, D.M., Weidmann, M., Matallana-Surget, S., Quilliam, R.S., 2021. Survival of human enteric and respiratory viruses on plastics in soil, freshwater, and marine environments. Environ. Res. 199, 111367. https://doi.org/10.1016/j.envres.2021.111367.

Mottier, A., Mouchet, F., Laplanche, C., Cadarsi, S., Lagier, L., Arnault, J.-C., Girard, H. A., León, V., Vázquez, E., Sarrieu, C., Pinelli, É., Gauthier, L., Flahaut, E., 2016. Surface area of carbon nanoparticles: A dose metric for a more realistic ecotoxicological assessment. Nano Lett. 16, 3514–3518. https://doi.org/10.1021/acs.nanolett.6b00348.

Muhammad, A., He, J., Yu, T., Sun, C., Shi, D., Jiang, Y., Xianyu, Y., Shao, Y., 2022. Dietary exposure of copper and zinc oxides

nanoparticles affect the fitness, enzyme activity, and microbial community of the model insect, silkworm *Bombyx mori*. Sci. Total Environ. 813, 152608. https://doi.org/10.1016/j.scitotenv.2021.152608.

Müller, T.G., Sakin, V., Müller, B., 2019. A spotlight on viruses — Application of click chemistry to visualize virus-cell interactions. Molecules 24, 481. https://doi.org/10.3390/molecules24030481.

Musee, N., Zvimba, J.N., Schaefer, L.M., Nota, N., Sikhwivhilu, L.M., Thwala, M., 2014. Fate and behavior of ZnO- and Ag-engineered nanoparticles and a bacterial viability assessment in a simulated wastewater treatment plant. J. Environ. Sci. Heal. A 49, 59–66. https://doi.org/10.1080/10934529.2013.824302.

Na, M., Nam, S.H., Moon, K., Kim, J., 2023. Development of a nano-QSAR model for predicting the toxicity of nano-metal oxide mixtures to *Aliivibrio fischeri*. Environ. Sci.: Nano, 10, 325–337. https://doi.org/10.1039/D2EN00672C.

Nakao, S., Akita, K., Ozaki, A., Masumoto, K., Okuda, T., 2021. Circulation of fibrous microplastic (microfiber) in sewage and sewage sludge treatment processes. Sci. Total Environ. 795, 148873. https://doi.org/10.1016/j.scitotenv.2021.148873.

Nasser, F., Lynch, I., 2016. Secreted protein eco-corona mediates uptake and impacts of polystyrene nanoparticles on *Daphnia magna*. J. Proteomics 137, 45–51. https://doi.org/10.1016/j.jprot.2015.09.005.

Navarro, A., Gómez, L., Sanseverino, I., Niegowska, M., Roka, E., Pedraccini, R., Vargha, M., Lettieri, T., 2021. SARS-CoV-2 detection in wastewater using multiplex quantitative PCR. Sci. Total Environ. 797, 148890. https://doi.org/10.1016/j.scitotenv.2021.148890.

Nunes, B.Z., Moreira, L.B., Xu, E.G., Castro, Í.B., 2023. A global snapshot of microplastic contamination in sediments and biota

of marine protected areas. Sci. Total Environ. 865, 161293. https://doi.org/10.1016/j.scitotenv.2022.161293.

Nur, Y., Lead, J.R., Baalousha, M., 2015. Evaluation of charge and agglomeration behavior of TiO_2 nanoparticles in ecotoxicological media. Sci. Total Environ. 535, 45–53. https://doi.org/10.1016/j.scitotenv.2014.11.057.

Nyoka, N.W.-K., Kanyile, S.N., Bredenhand, E., Prinsloo, G.J., Voua Otomo, P., 2018. Biochar alleviates the toxicity of imidacloprid and silver nanoparticles (AgNPs) to *Enchytraeus albidus* (Oligochaeta). Environ. Sci. Pollut. Res. 25, 10937–10945. https://doi.org/10.1007/s11356-018-1383-x.

O'Brien, S., Okoffo, E.D., O'Brien, J.W., Ribeiro, F., Wang, X., Wright, S.L., Samanipour, S., Rauert, C., Toapanta, T.Y.A., Albarracin, R., Thomas, K.V., 2020. Airborne emissions of microplastic fibres from domestic laundry dryers. Sci. Total Environ. 747, 141175. https://doi.org/10.1016/j.scitotenv.2020.141175.

OECD, 2014. Guidance Document on the Validation of (Quantitative) Structure-Activity Relationship [(Q)SAR] Models, OECD Series on Testing and Assessment. OECD. https://doi.org/10.1787/9789264085442-en.

Oksel Karakus, C., Bilgi, E., Winkler, D.A., 2021. Biomedical nanomaterials: Applications, toxicological concerns, and regulatory needs. Nanotoxicology 15, 331–351. https://doi.org/10.1080/17435390.2020.1860265.

Olasupo, S.B., Uzairu, A., Shallangwa, G.A., Uba, S., 2020. Chemoinformatic studies on some inhibitors of dopamine transporter and the receptor targeting schizophrenia for developing novel antipsychotic agents. Heliyon 6, e04464. https://doi.org/10.1016/j.heliyon.2020.e04464.

Palmieri, V., Papi, M., 2020. Can graphene take part in the fight against COVID-19? Nano Today 33, 100883. https://doi.org/10.

1016/j.nantod.2020.100883.

Pan, B., Xing, B., 2008. Adsorption mechanisms of organic chemicals on carbon nanotubes. Environ. Sci. Technol. 42, 9005–9013. https://doi.org/10.1021/es801777n.

Parsai, T., Kumar, A., 2019. Understanding effect of solution chemistry on heteroaggregation of zinc oxide and copper oxide nanoparticles. Chemosphere 235, 457–469. https://doi.org/10.1016/j.chemosphere.2019.06.171.

Parsai, T., Kumar, A., 2020. Stability and characterization of mixture of three particle system containing ZnO-CuO nanoparticles and clay. Sci. Total Environ. 740, 140095. https://doi.org/10.1016/j.scitotenv.2020.140095.

Patel, K.D., Singh, R.K., Kim, H.-W., 2019. Carbon-based nanomaterials as an emerging platform for theranostics. Mater. Horiz. 6, 434–469. https://doi.org/10.1039/c8mh00966j.

Patil, S.M., Rane, N.R., Bankole, P.O., Krishnaiah, P., Ahn, Y., Park, Y.-K., Yadav, K.K., Amin, M.A., Jeon, B.-H., 2022. An assessment of micro- and nanoplastics in the biosphere: A review of detection, monitoring, and remediation technology. Chem. Eng. J. 430, 132913. https://doi.org/10.1016/j.cej.2021.132913.

Patton, T., Barrett, J., Brennan, J., Moran, N., 2006. Use of a spectrophotometric bioassay for determination of microbial sensitivity to manuka honey. J. Microbiol. Methods 64, 84–95. https://doi.org/10.1016/j.mimet.2005.04.007.

Paul, D., Kolar, P., Hall, S.G., 2021. A review of the impact of environmental factors on the fate and transport of coronaviruses in aqueous environments. npj Clean Water 4, 7. https://doi.org/10.1038/s41545-020-00096-w.

Peijnenburg, W.J.G.M., Baalousha, M., Chen, J., Chaudry, Q., Von Der Kammer, F., Kuhlbusch, T.A.J., Lead, J., Nickel, C., Quik,

J.T.K., Renker, M., Wang, Z., Koelmans, A.A., 2015. A review of the properties and processes determining the fate of engineered nanomaterials in the aquatic environment. Crit. Rev. Environ. Sci. Technol. 45, 2084–2134. https://doi.org/10.1080/10643389.2015.1010430.

Pérez Santín, E., Rodríguez Solana, R., González García, M., Del García Suárez, M.M., Blanco Díaz, G.D., Cima Cabal, M.D., Moreno Rojas, J.M., López Sánchez, J.I., 2021. Toxicity prediction based on artificial intelligence: A multidisciplinary overview. WIREs Comput. Mol. Sci. 11, e1516. https://doi.org/10.1002/wcms.1516.

Pérez-Hernández, H., Pérez-Moreno, A., Sarabia-Castillo, C.R., García-Mayagoitia, S., Medina-Pérez, G., López-Valdez, F., Campos-Montiel, R.G., Jayanta-Kumar, P., Fernández-Luqueño, F., 2021. Ecological drawbacks of nanomaterials produced on an industrial scale: Collateral effect on human and environmental health. Water Air Soil Pollut. 232, 435. https://doi.org/10.1007/s11270-021-05370-2.

Persson, L., Carney Almroth, B.M., Collins, C.D., Cornell, S., de Wit, C.A., Diamond, M.L., Fantke, P., Hassellöv, M., MacLeod, M., Ryberg, M.W., Søgaard Jørgensen, P., Villarrubia-Gómez, P., Wang, Z., Hauschild, M.Z., 2022. Outside the safe operating space of the planetary boundary for novel entities. Environ. Sci. Technol. 56, 1510–1521. https://doi.org/10.1021/acs.est.1c04158.

Persson, L.M., Breitholtz, M., Cousins, I.T., de Wit, C.A., MacLeod, M., McLachlan, M.S., 2013. Confronting unknown planetary boundary threats from chemical pollution. Environ. Sci. Technol. 47, 12619–12622. https://doi.org/10.1021/es402501c.

Pikula, K., Johari, S.A., Santos-Oliveira, R., Golokhvast, K., 2022. Individual and binary mixture toxicity of five nanoparticles in marine microalga *Heterosigma akashiwo*. Int. J. Mol. Sci. 23, 990. https://doi.org/10.3390/ijms23020990.

Puzyn, T., Rasulev, B., Gajewicz, A., Hu, X., Dasari, T.P., Michalkova, A., Hwang, H.-M., Toropov, A., Leszczynska, D., Leszczynski, J., 2011. Using nano-QSAR to predict the cytotoxicity of metal oxide nanoparticles. Nat. Nanotechnol. 6, 175–178. https://doi.org/10.1038/nnano.2011.10.

Qi, P., Qiu, L., Feng, D., Gu, Z., Guo, B., Yan, X., 2023. Distinguish the toxic differentiations between acute exposure of micro- and nano-plastics on bivalves: An integrated study based on transcriptomic sequencing. Aquat. Toxicol. 254, 106367. https://doi.org/10.1016/j.aquatox.2022.106367.

Qi, Z., Hou, L., Zhu, D., Ji, R., Chen, W., 2014. Enhanced transport of phenanthrene and 1-naphthol by colloidal graphene oxide nanoparticles in saturated soil. Environ. Sci. Technol. 48, 10136–10144. https://doi.org/10.1021/es500833z.

Ragab, D., Salah Eldin, H., Taeimah, M., Khattab, R., Salem, R., 2020. The COVID-19 cytokine storm; What we know so far. Front. Immunol. 11, 1446. https://doi.org/10.3389/fimmu.2020.01446.

Rai, P.K., Lee, J., Brown, R.J.C., Kim, K.H., 2021. Environmental fate, ecotoxicity biomarkers, and potential health effects of micro- and nano-scale plastic contamination. J. Hazard. Mater. 403, 123910. https://doi.org/10.1016/j.jhazmat.2020.123910.

Randazzo, W., Truchado, P., Cuevas-Ferrando, E., Simón, P., Allende, A., Sánchez, G., 2020. SARS-CoV-2 RNA in wastewater anticipated COVID-19 occurrence in a low prevalence area. Water Res. 181, 115942. https://doi.org/10.1016/j.watres.2020.115942.

Razzini, K., Castrica, M., Menchetti, L., Maggi, L., Negroni, L., Orfeo, N.V., Pizzoccheri, A., Stocco, M., Muttini, S., Balzaretti, C.M., 2020. SARS-CoV-2 RNA detection in the air and on surfaces in the COVID-19 ward of a hospital in Milan, Italy. Sci. Total Environ. 742, 140540. https://doi.org/10.1016/j.scitotenv.2020.

140540.

Reddy, N., Lynch, B., Gujral, J., Karnik, K., 2023. Alternatives to animal testing in toxicity testing: Current status and future perspectives in food safety assessments. Food Chem. Toxicol. 179, 113944. https://doi.org/10.1016/j.fct.2023.113944.

Rezania, S., Park, J., Md Din, M.F., Mat Taib, S., Talaiekhozani, A., Kumar Yadav, K., Kamyab, H., 2018. Microplastics pollution in different aquatic environments and biota: A review of recent studies. Mar. Pollut. Bull. 133, 191–208. https://doi.org/10.1016/j.marpolbul.2018.05.022.

Rider, C.V., Simmons, J.E., 2018. Chemical mixtures and combined chemical and nonchemical stressors. Cham: Springer International Publishing.

Robertson, M.P., Igel, H., Baertsch, R., Haussler, D., Ares, M., Scott, W.G., 2004. The structure of a rigorously conserved RNA element within the SARS virus genome. PLoS Biol. 3, e5. https://doi. org/10.1371/journal.pbio.0030005.

Rockström, J., Steffen, W., Noone, K., Persson, Å., Chapin, F.S.I., Lambin, E., Lenton, T.M., Scheffer, M., Folke, C., Schellnhuber, H.J., Nykvist, B., de Wit, C.A., Hughes, T., van der Leeuw, S., Rodhe, H., Sörlin, S., Snyder, P.K., Costanza, R., Svedin, U., Falkenmark, M., Karlberg, L., Corell, R.W., Fabry, V.J., Hansen, J., Walker, B., Liverman, D., Richardson, K., Crutzen, P., Foley, J., 2009. Planetary boundaries: Exploring the safe operating space for humanity. Ecol. Soc. 14, 32. https://doi.org/10.5751/ES-03180-140232.

Rodrigues, C.C., Salla, R.F., Rocha, T.L., 2023. Bioaccumulation and ecotoxicological impact of micro(nano)plastics in aquatic and land snails: Historical review, current research and emerging trends. J. Hazard. Mater. 444, 130382. https://doi.org/10.1016/j.jhazmat.2022.130382.

Roje, Ž., Ilić, K., Galić, E., Pavičić, I., Turčić, P., Stanec, Z., Vrček, I.V., 2019. Synergistic effects of parabens and plastic nanoparticles on proliferation of human breast cancer cells. Arh. Hig. Rada. Toksikol. 70, 310–314. https://doi.org/10.2478/aiht-2019-70-3372.

Romera-Castillo, C., Lucas, A., Mallenco-Fornies, R., Briones-Rizo, M., Calvo, E., Pelejero, C., 2023. Abiotic plastic leaching contributes to ocean acidification. Sci. Total Environ. 854, 158683. https://doi. org/10.1016/j.scitotenv.2022.158683.

Rompelberg, C., Heringa, M.B., van Donkersgoed, G., Drijvers, J., Roos, A., Westenbrink, S., Peters, R., van Bemmel, G., Brand, W., Oomen, A.G., 2016. Oral intake of added titanium dioxide and its nanofraction from food products, food supplements and toothpaste by the Dutch population. Nanotoxicology 10, 1404–1414. https://doi.org/10.1080/17435390.2016.1222457.

Roscher, L., Fehres, A., Reisel, L., Halbach, M., Scholz-Böttcher, B., Gerriets, M., Badewien, T.H., Shiravani, G., Wurpts, A., Primpke, S., Gerdts, G., 2021. Microplastic pollution in the Weser estuary and the German North Sea. Environ. Pollut. 288, 117681. https://doi.org/10.1016/j.envpol.2021.117681.

Rosenfeldt, R.R., Seitz, F., Haigis, A.-C., Höger, J., Zubrod, J.P., Schulz, R., Bundschuh, M., 2016. Nanosized titanium dioxide influences copper-induced toxicity during aging as a function of environmental conditions. Environ. Toxicol. Chem. 35, 1766–1774. https://doi.org/10.1002/etc.3325.

Roy, J., Ojha, P.K., Roy, K., 2019. Risk assessment of heterogeneous TiO_2-based engineered nanoparticles (NPs): A QSTR approach using simple periodic table based descriptors. Nanotoxicology 13, 701–716. https://doi.org/10.1080/17435390.2019.1593543.

Roy, K., Kar, S., Das, R.N., 2015. A Primer on QSAR/QSPR Modeling. Cham: Springer International Publishing AG. https://doi.org/10.

1007/978-3-319-17281-1.

Saavedra, J., Stoll, S., Slaveykova, V.I., 2019. Influence of nanoplastic surface charge on eco-corona formation, aggregation and toxicity to freshwater zooplankton. Environ. Pollut. 252, 715–722. https://doi.org/10.1016/j.envpol.2019.05.135.

Saingam, P., Li, B., Nguyen Quoc, B., Jain, T., Bryan, A., Winkler, M.K.H., 2023. Wastewater surveillance of SARS-CoV-2 at intra-city level demonstrated high resolution in tracking COVID-19 and calibration using chemical indicators. Sci. Total Environ. 866, 161467. https://doi.org/10.1016/j.scitotenv.2023.161467.

Sala-Comorera, L., Reynolds, L.J., Martin, N.A., O'Sullivan, J.J., Meijer, W.G., Fletcher, N.F., 2021. Decay of infectious SARS-CoV-2 and surrogates in aquatic environments. Water Res. 201, 117090. https://doi.org/10.1016/j.watres.2021.117090.

Sanchez-Galan, J.E., Ureña, G., Escovar, L.F., Fabrega-Duque, J.R., Coles, A., Kurt, Z., 2021. Challenges to detect SARS-CoV-2 on environmental media, the need and strategies to implement the detection methodologies in wastewaters. J. Environ. Chem. Eng. 9, 105881. https://doi.org/10.1016/j.jece.2021.105881.

Sánchez-López, E., Gomes, D., Esteruelas, G., Bonilla, L., Lopez-Machado, A.L., Galindo, R., Cano, A., Espina, M., Ettcheto, M., Camins, A., Silva, A.M., Durazzo, A., Santini, A., Garcia, M.L., Souto, E.B., 2020. Metal-based nanoparticles as antimicrobial agents: An overview. Nanomaterials 10, 292. https://doi.org/10.3390/nano10020292.

Sanchís, J., Jiménez-Lamana, J., Abad, E., Szpunar, J., Farré, M., 2020. Occurrence of cerium-, titanium-, and silver-bearing nanoparticles in the Besòs and Ebro Rivers. Environ. Sci. Technol. 54, 3969–3978. https://doi.org/10.1021/acs.est.9b05996.

Saravanan, A., Kumar, P.S., Hemavathy, R.V., Jeevanantham, S., Jawahar, M.J., Neshaanthini, J.P., Saravanan, R., 2022. A review on synthesis methods and recent applications of nanomaterial in wastewater treatment: Challenges and future perspectives. Chemosphere 307, 135713. https://doi.org/10.1016/j.chemosphere.2022.135713.

Savastano, A., Ibáñez de Opakua, A., Rankovic, M., Zweckstetter, M., 2020. Nucleocapsid protein of SARS-CoV-2 phase separates into RNA-rich polymerase-containing condensates. Nat. Commun. 11, 6041. https://doi.org/10.1038/s41467-020-19843-1.

Sayadi, M.H., Pavlaki, M.D., Loureiro, S., Martins, R., Tyler, C.R., Mansouri, B., Kharkan, J., Shekari, H., 2022. Co-exposure of Zinc oxide nanoparticles and multi-layer graphenes in blackfish (*Capoeta fusca*): Evaluation of lethal, behavioural, and histopathological effects. Ecotoxicology 31, 425–439. https://doi.org/10.1007/s10646-022-02521-x.

Sayadi, M.H., Pavlaki, M.D., Martins, R., Mansouri, B., Tyler, C.R., Kharkan, J., Shekari, H., 2021. Bioaccumulation and toxicokinetics of zinc oxide nanoparticles (ZnO NPs) co-exposed with graphene nanosheets (GNs) in the blackfish (*Capoeta fusca*). Chemosphere 269, 128689. https://doi.org/10.1016/j.chemosphere.2020.128689.

Sellami, B., Mezni, A., Khazri, A., Bouzidi, I., Saidani, W., Sheehan, D., Beyrem, H., 2017. Toxicity assessment of ZnO-decorated Au nanoparticles in the mediterranean clam *Ruditapes decussatus*. Aquat. Toxicol. 188, 10–19. https://doi.org/10.1016/j.aquatox.2017.04.005.

Serrano-Aroca, Á., Takayama, K., Tuñón-Molina, A., Seyran, M., Hassan, S.S., Pal Choudhury, P., Uversky, V.N., Lundstrom, K., Adadi, P., Palù, G., Aljabali, A.A.A., Chauhan, G., Kandimalla, R., Tambuwala, M.M., Lal, A., Abd El-Aziz, T.M., Sherchan, S., Barh, D., Redwan, E.M., Bazan, N.G., Mishra, Y.K., Uhal, B.D., Brufsky,

A., 2021. Carbon-based nanomaterials: Promising antiviral agents to combat COVID-19 in the microbial-resistant era. ACS Nano 15, 8069–8086. https://doi.org/10.1021/acsnano.1c00629.

Shao, B., Liu, Z., Tang, L., Liu, Y., Liang, Q., Wu, T., Pan, Y., Zhang, X., Tan, X., Yu, J., 2022. The effects of biochar on antibiotic resistance genes (ARGs) removal during different environmental governance processes: A review. J. Hazard. Mater. 435, 129067. https://doi. org/10.1016/j.jhazmat.2022.129067.

Shao, B., Wang, J., Liu, Z., Zeng, G., Tang, L., Liang, Q., He, Q., Wu, T., Liu, Y., Yuan, X., 2020. $Ti_3C_2T_x$ MXene decorated black phosphorus nanosheets with improved visible-light photocatalytic activity: Experimental and theoretical studies. J. Mater. Chem. A 8, 5171–5185. https://doi.org/10.1039/c9ta13610j.

Sharma, B., Tiwari, S., Kumawat, K.C., Cardinale, M., 2023. Nano-biofertilizers as bio-emerging strategies for sustainable agriculture development: Potentiality and their limitations. Sci. Total Environ. 860, 160476. https://doi.org/10.1016/j.scitotenv.2022.160476.

Sheng, Y., Liu, Y., Wang, K., Cizdziel, J.V., Wu, Y., Zhou, Y., 2021. Ecotoxicological effects of micronized car tire wear particles and their heavy metals on the earthworm (*Eisenia fetida*) in soil. Sci. Total Environ. 793, 148613. https://doi.org/10.1016/j.scitotenv.2021.148613.

Shi, X., Wang, X., Huang, R., Tang, C., Hu, C., Ning, P., Wang, F., 2022. Cytotoxicity and genotoxicity of polystyrene micro- and nanoplastics with different size and surface modification in A549 cells. Int. J. Nanomedicine 17, 4509–4523. https://doi.org/10.2147/IJN.S381776.

Shin, M.D., Shukla, S., Chung, Y.H., Beiss, V., Chan, S.K., Ortega-

Rivera, O.A., Wirth, D. M., Chen, A., Sack, M., Pokorski, J.K., Steinmetz, N.F., 2020. COVID-19 vaccine development and a potential nanomaterial path forward. Nat. Nanotechnol. 15, 646–655. https://doi.org/10.1038/s41565-020-0737-y.

Simelane, S., Dlamini, L.N., 2019. An investigation of the fate and behaviour of a mixture of WO_3 and TiO_2 nanoparticles in a wastewater treatment plant. J. Environ. Sci. 76, 37–47. https://doi.org/10.1016/j.jes.2018.03.018.

Singh, D., Kumar, A., 2020. Binary mixture of nanoparticles in sewage sludge: Impact on spinach growth. Chemosphere 254, 126794. https://doi.org/10.1016/j.chemosphere.2020.126794.

Singh, N.B., Chaudhary, R.G., Desimone, M.F., Agrawal, A., Shukla, S.K., 2023. Green synthesized nanomaterials for safe technology in sustainable agriculture. Curr. Pharm. Biotechnol. 24, 61–85. https://doi.org/10.2174/1389201023666220608113924.

Skiba, E., Pietrzak, M., Glińska, S., Wolf, W.M., 2021. The combined effect of ZnO and CeO_2 nanoparticles on *Pisum sativum* L.: A photosynthesis and nutrients uptake study. Cells 10, 3105. https://doi.org/10.3390/cells10113105.

Slot, E., Hogema, B.M., Reusken, C.B.E.M., Reimerink, J.H., Molier, M., Karregat, J.H.M., IJlst, J., Novotný, V.M.J., van Lier, R.A.W., Zaaijer, H.L., 2020. Low SARS-CoV-2 seroprevalence in blood donors in the early COVID-19 epidemic in the Netherlands. Nat. Commun. 11, 5744. https://doi.org/10.1038/s41467-020-19481-7.

Snape, M.D., Viner, R.M., 2020. COVID-19 in children and young people. Science 370, 286–288. https://doi.org/10.1126/science.abd6165.

Stadnytskyi, V., Bax, C.E., Bax, A., Anfinrud, P., 2020. The airborne lifetime of small speech droplets and their potential importance in SARS-CoV-2 transmission. Proc. Natl. Acad. Sci. 117, 11875–

11877. https://doi.org/10.1073/pnas.2006874117.

Steffan, J.J., Derby, J.A., Brevik, E.C., 2020. Soil pathogens that may potentially cause pandemics, including severe acute respiratory syndrome (SARS) coronaviruses. Curr. Opin. Environ. Sci. Health 17, 35–40. https://doi.org/10.1016/j.coesh.2020.08.005.

Steffen, W., Richardson, K., Rockström, J., Cornell, S.E., Fetzer, I., Bennett, E.M., Biggs, R., Carpenter, S.R., de Vries ,W., de Wit, C.A., Folke, C., Gerten, D., Heinke, J., Mace, G.M., Persson, L.M., Ramanathan, V., Reyers, B., Sörlin, S., 2015. Sustainability. Planetary boundaries: Guiding human development on a changing planet. Science 347, 1259855. https://doi.org/10.1126/science.1259855.

Stuart, E.J.E., Compton, R.G., 2015. Nanoparticles-emerging contaminants. In environmental analysis by electrochemical sensors and biosensors; Moretto, L.M., Kalcher, K., Eds.; Springer; Nanostructure science and technology, pp 855–878. https://doi.org/10.1007/978-1-4939-1301-5_8.

Sun, N., Shi, H., Li, X., Gao, C., Liu, R., 2023. Combined toxicity of micro/nanoplastics loaded with environmental pollutants to organisms and cells: Role, effects, and mechanism. Environ. Int. 171, 107711. https://doi.org/10.1016/j.envint.2022.107711.

Sun, Q., Xie, H.-B., Chen, J., Li, X., Wang, Z., Sheng, L., 2013. Molecular dynamics simulations on the interactions of low molecular weight natural organic acids with C_{60}. Chemosphere 92, 429–434. https://doi.org/10.1016/j.chemosphere.2013.01.039.

Sun, S., Shi, W., Tang, Y., Han, Y., Du, X., Zhou, W., Zhang, W., Sun, C., Liu, G., 2021. The toxic impacts of microplastics (MPs) and polycyclic aromatic hydrocarbons (PAHs) on haematic parameters in a marine bivalve species and their potential mechanisms of action. Sci. Total Environ. 783, 147003. https://

doi.org/10.1016/j.scitotenv.2021.147003.

Sundaram, B., Kumar, A., 2017. Long-term effect of metal oxide nanoparticles on activated sludge. Water Sci. Technol. 75, 462–473. https://doi.org/10.2166/wst.2016.541.

Talebian, S., Wallace, G.G., Schroeder, A., Stellacci, F., Conde, J., 2020. Nanotechnology-based disinfectants and sensors for SARS-CoV-2. Nat. Nanotechnol. 15, 618–621. https://doi.org/10.1038/s41565-020-0751-0.

Tiede, K., Hanssen, S.F., Westerhoff, P., Fern, G.J., Hankin, S.M., Aitken, R.J., Chaudhry, Q., Boxall, A.B., 2016. How important is drinking water exposure for the risks of engineered nanoparticles to consumers? Nanotoxicology 10, 102–110. https://doi.org/10.3109/17435390.2015.1022888.

Tong, T., Fang, K., Thomas, S.A., Kelly, J.J., Gray, K.A., Gaillard, J.-F., 2014. Chemical interactions between nano-ZnO and nano-TiO_2 in a natural aqueous medium. Environ. Sci. Technol. 48, 7924–7932. https://doi.org/10.1021/es501168p.

Tong, T., Wilke, C.M., Wu, J., Binh, C.T.T., Kelly, J.J., Gaillard, J.-F., Gray, K.A., 2015. Combined toxicity of nano-ZnO and nano-TiO_2: From single- to multinanomaterial systems. Environ. Sci. Technol. 49, 8113–8123. https://doi.org/10.1021/acs.est.5b02148.

Topol, E.J., 2020. COVID-19 can affect the heart. Science 370, 408–409. https://doi.org/10.1126/science.abe2813.

Tou, F., Wu, J., Fu, J., Niu, Z., Liu, M., Yang, Y., 2021. Titanium and zinc-containing nanoparticles in estuarine sediments: Occurrence and their environmental implications. Sci. Total Environ. 754, 142388. https://doi.org/10.1016/j.scitotenv.2020.142388.

Trinh, T.X., Kim, J., 2021. Status quo in data availability and

predictive models of nano-mixture toxicity. Nanomaterials 11, 124. https://doi.org/10.3390/nano11010124.

Trinh, T.X., Seo, M., Yoon, T.H., Kim, J., 2022. Developing random forest based QSAR models for predicting the mixture toxicity of TiO_2 based nano-mixtures to *Daphnia magna*. NanoImpact 25, 100383. https://doi.org/10.1016/j.impact.2022.100383.

Tropsha, A., 2010. Best practices for QSAR model development, validation, and exploitation. Mol. Inform. 29, 476–488. https://doi.org/10.1002/minf.201000061.

Turner, J.S., Kim, W., Kalaidina, E., Goss, C.W., Rauseo, A.M., Schmitz, A.J., Hansen, L., Haile, A., Klebert, M.K., Pusic, I., O'Halloran, J.A., Presti, R.M., Ellebedy, A.H., 2021. SARS-CoV-2 infection induces long-lived bone marrow plasma cells in humans. Nature 595, 421–425. https://doi.org/10.1038/s41586-021-03647-4.

UNEP, 2016. Marine plastic debris and microplastics — Global lessons and research to inspire action and guide policy change. United Nations Environment Programme, Nairobi. https://doi.org/10. 13140/RG.2.2.30493.51687.

Upfold, N.S., Luke, G.A., Knox, C., 2021. Occurrence of human enteric viruses in water sources and shellfish: A focus on Africa. Food Environ. Virol. 13, 1–31. https://doi.org/10.1007/s12560-020-09456-8.

Van Leeuwen, C.J., Bro-Rasmussen, F., Feijtel, T.C., Arndt, R., Bussian, B.M., Calamari, D., Glynn, P., Grandy, N.J., Hansen, B., van Hemmen, J.J., Hurst, P., King, N., Koch, R., Müller, M., Solbé, J.F., Speijers, G.A., Vermeire, T., 1996. Risk assessment and management of new and existing chemicals. Environ. Toxicol. Phar. 2, 243–299. https://doi.org/10.1016/s1382-6689(96)00072-5.

Verma, A., Uzun, O., Hu, Y., Hu, Y., Han, H.-S., Watson, N., Chen, S.,

Irvine, D.J., Stellacci, F., 2008. Surface-structure-regulated cell-membrane penetration by monolayer-protected nanoparticles. Nat. Mater. 7, 588–595. https://doi.org/10.1038/nmat2202.

Vermisoglou, E., Panáček, D., Jayaramulu, K., Pykal, M., Frébort, I., Kolář, M., Hajdúch, M., Zbořil, R., Otyepka, M., 2020. Human virus detection with graphene-based materials. Biosens. Bioelectron. 166, 112436. https://doi.org/10.1016/j.bios.2020.112436.

Vijver, M.G., Elliott, E.G., Peijnenburg, W.J.G.M., de Snoo, G.R., 2011. Response predictions for organisms water-exposed to metal mixtures: A meta-analysis. Environ. Toxicol. Chem. 30, 1482–1487. https://doi.org/10.1002/etc.499.

Vijver, M.G., Peijnenburg, W.J.G.M., de Snoo, G.R., 2010. Toxicological mixture models are based on inadequate assumptions. Environ. Sci. Technol. 44, 4841–4842. https://doi.org/10.1021/es1001659.

Visalli, G., Facciolà, A., Pruiti Ciarello, M., De Marco, G., Maisano, M., Di Pietro, A., 2021. Acute and sub-chronic effects of microplastics (3 and 10 μm) on the human intestinal cells HT-29. Int. J. Environ. Res. Public Health 18, 5833. https://doi.org/10.3390/ijerph18115833.

Walker, J.D., Enache, M., Dearden, J.C., 2003. Quantitative cationic–activity relationships for predicting toxicity of metals. Environ. Toxicol. Chem. 22, 1916–1935. https://doi.org/10.1897/02-568.

Wang, J., Peng, C., Dai, Y., Li, Y., Jiao, S., Ma, X., Liu, X., Wang, L., 2022. Slower antibiotics degradation and higher resistance genes enrichment in plastisphere. Water Res. 222, 118920. https://doi.org/10.1016/j.watres.2022.118920.

Wang, M., Yu, H.L., Chen, Y., Huang, M.X., 2021. Machine learning assisted screening of non-rare-earth elements for Mg alloys with

low stacking fault energy. Comp. Mater. Sci. 196, 110544. https://doi.org/10.1016/j.commatsci.2021.110544.

Wang, Q., Li, Y., Lung, D.C., Chan, P.-T., Dung, C.-H., Jia, W., Miao, T., Huang, J., Chen, W., Wang, Z., Leung, K.-M., Lin, Z., Wong, D., Tse, H., Wong, S.C.Y., Choi, G.K.-Y., Lam, J,Y.-W., To, K.K.-W., Cheng, V.C.-C., Yuen, K.-Y., 2022. Aerosol transmission of SARS-CoV-2 due to the chimney effect in two high-rise housing drainage stacks. J. Hazard. Mater. 421, 126799. https://doi.org/10.1016/j. jhazmat.2021.126799.

Wang, W., Do, A.T.N., Kwon, J.-H., 2022. Ecotoxicological effects of micro- and nanoplastics on terrestrial food web from plants to human beings. Sci. Total Environ. 834, 155333. https://doi. org/10.1016/j.scitotenv.2022.155333.

Wang, X., Ren, X.-M., He, H., Li, F., Liu, K., Zhao, F., Hu, H., Zhang, P., Huang, B., Pan, X., 2023. Cytotoxicity and pro-inflammatory effect of polystyrene nano-plastic and micro-plastic on RAW264.7 cells. Toxicology 484, 153391. https://doi.org/10. 1016/j.tox.2022. 153391.

Wang, Y., Chen, J., Wei, X., Hernandez Maldonado, A.J., Chen, Z., 2017. Unveiling adsorption mechanisms of organic pollutants onto carbon nanomaterials by density functional theory computations and linear free energy relationship modeling. Environ. Sci. Technol. 51, 11820–11828. https://doi.org/10.1021/ acs.est.7b02707.

Wang, Y., Chen, X., 2020. A joint optimization QSAR model of fathead minnow acute toxicity based on a radial basis function neural network and its consensus modeling. RSC Adv. 10, 21292–21308. https://doi.org/10.1039/d0ra02701d.

Wang, Z., Jin, S., Zhang, F., Wang, D., 2020. Combined toxicity of TiO_2 nanospherical particles and TiO_2 nanotubes to two micro-algae with different morphology. Nanomaterials 10, 2559.

https://doi.org/10.3390/nano10122559.

Wang, Z., Vijver, M.G., Peijnenburg, W.J.G.M., 2018. Multiscale coupling strategy for nano ecotoxicology prediction. Environ. Sci. Technol. 52, 7598–7600. https://doi.org/10.1021/acs.est.8b02895.

Wang, Z., Zhang, F., Vijver, M.G., Peijnenburg, W.J.G.M., 2021. Graphene nanoplatelets and reduced graphene oxide elevate the microalgal cytotoxicity of nano-zirconium oxide. Chemosphere 276, 130015. https://doi.org/10.1016/j.chemosphere.2021.130015.

Wheeler, K.E., Chetwynd, A.J., Fahy, K.M., Hong, B.S., Tochihuitl, J.A., Foster, L.A., Lynch, I., 2021. Environmental dimensions of the protein corona. Nat. Nanotechnol. 16, 617–629. https://doi.org/10.1038/s41565-021-00924-1.

Wiktorczyk-Kapischke, N., Grudlewska-Buda, K., Wałecka-Zacharska, E., Kwiecińska-Piróg, J., Radtke, L., Gospodarek-Komkowska, E., Skowron, K., 2021. SARS-CoV-2 in the environment — Non-droplet spreading routes. Sci. Total Environ. 770, 145260. https://doi.org/10.1016/j.scitotenv.2021.145260.

Wilke, C.M., Tong, T., Gaillard, J.-F., Gray, K.A., 2016. Attenuation of microbial stress due to nano-Ag and nano-TiO_2 interactions under dark conditions. Environ. Sci. Technol. 50, 11302–11310. https://doi.org/10.1021/acs.est.6b02271.

Wilke, C.M., Wunderlich, B., Gaillard, J.-F., Gray, K.A., 2018. Synergistic bacterial stress results from exposure to nano-Ag and nano-TiO_2 mixtures under light in environmental media. Environ. Sci. Technol. 52, 3185–3194. https://doi.org/10.1021/acs.est.7b05629.

Wu, S., Gaillard, J.-F., Gray, K.A., 2021. The impacts of metal-based engineered nanomaterial mixtures on microbial systems: A

review. Sci. Total Environ. 780, 146496. https://doi.org/10.1016/j.scitotenv.2021.146496.

Wu, S., Zhang, S., Gong, Y., Shi, L., Zhou, B., 2020. Identification and quantification of titanium nanoparticles in surface water: A case study in Lake Taihu, China. J. Hazard. Mater. 382, 121045. https://doi.org/10.1016/j.jhazmat.2019.121045.

Wu, T., He, Q., Liu, Z., Shao, B., Liang, Q., Pan, Y., Huang, J., Peng, Z., Liu, Y., Zhao, C., Yuan, X., Tang, L., Gong, S., 2022. Tube wall delamination engineering induces photogenerated carrier separation to achieve photocatalytic performance improvement of tubular g-C_3N_4. J. Hazard. Mater. 424, 127177. https://doi.org/10.1016/j.jhazmat.2021.127177.

Wyrzykowska, E., Mikolajczyk, A., Lynch, I., Jeliazkova, N., Kochev, N., Sarimveis, H., Doganis, P., Karatzas, P., Afantitis, A., Melagraki, G., Serra, A., Greco, D., Subbotina, J., Lobaskin, V., Bañares, M.A., Valsami-Jones, E., Jagiello, K., Puzyn, T., 2022. Representing and describing nanomaterials in predictive nanoinformatics. Nat. Nanotechnol. 17, 924–932. https://doi.org/10.1038/s41565-022-01173-6.

Xia, J., Zhao, H.Z., Lu, G.H., 2013. Effects of selected metal oxide nanoparticles on multiple biomarkers in *Carassius auratus*. Biomed. Environ. Sci. 26, 742–749. https://doi.org/10.3967/0895-3988.2013.09.005.

Xiao, Y., Peijnenburg, W.J.G.M., Chen, G., Vijver, M.G., 2016. Toxicity of copper nanoparticles to *Daphnia magna* under different exposure conditions. Sci. Total Environ. 563–564, 81–88. https://doi.org/10.1016/j.scitotenv.2016.04.104.

Xin, X., Chen, B., Yang, M., Gao, S., Wang, H., Gu, W., Li, X., Zhang, B., 2023. A critical review on the interaction of polymer particles and co-existing contaminants: Adsorption mechanism, exposure factors, effects on plankton species. J. Hazard. Mater. 445,

130463. https://doi.org/10.1016/j.jhazmat.2022.130463.

Xu, J.-L., Lin, X., Wang, J.J., Gowen, A.A., 2022. A review of potential human health impacts of micro- and nanoplastics exposure. Sci. Total Environ. 851, 158111. https://doi.org/10.1016/j.scitotenv. 2022.158111.

Xu, L., Wang, Z., Zhao, J., Lin, M., Xing, B., 2020. Accumulation of metal-based nanoparticles in marine bivalve mollusks from offshore aquaculture as detected by single particle ICP-MS. Environ. Pollut. 260, 114043. https://doi.org/10.1016/j.envpol. 2020.114043.

Xu, M., Yang, H., Liu, G., Tang, Y., Li, W., 2022. In silico prediction of chemical aquatic toxicity by multiple machine learning and deep learning approaches. J. Appl. Toxicol. 42, 1766–1776. https://doi.org/10.1002/jat.4354.

Yang, K., Xing, B., 2010. Adsorption of organic compounds by carbon nanomaterials in aqueous phase: Polanyi theory and its application. Chem. Rev. 110, 5989–6008. https://doi.org/10.1021/cr100059s.

Yang, L., Chen, P., He, K., Wang, R., Chen, G., Shan, G., Zhu, L., 2022. Predicting bioconcentration factor and estrogen receptor bioactivity of bisphenol a and its analogues in adult zebrafish by directed message passing neural networks. Environ. Int. 169, 107536. https://doi.org/10.1016/j.envint.2022.107536.

Yang, L., Yan, W., Wang, H., Zhuang, H., Zhang, J., 2017. Shell thickness-dependent antibacterial activity and biocompatibility of gold@silver core–shell nanoparticles. RSC Adv. 7, 11355–11361. https://doi.org/10.1039/c7ra00485k.

Yang, Q., Zhang, L., Ben, A., Wu, N., Yi, Y., Jiang, L., Huang, H., Yu, Y., 2018. Effects of dispersible MoS_2 nanosheets and nano-silver coexistence on the metabolome of yeast. Chemosphere 198, 216–225. https://doi.org/10.1016/j.chemosphere.2018.01.140.

Ye, N., Wang, Z., Wang, S., Peijnenburg, W.J.G.M., 2018. Toxicity of mixtures of zinc oxide and graphene oxide nanoparticles to aquatic organisms of different trophic level: Particles outperform dissolved ions. Nanotoxicology 12, 423–438. https://doi.org/10.1080/17435390.2018.1458342.

Yin, J., Huang, G., An, C., Feng, R., 2022. Nanocellulose enhances the dispersion and toxicity of ZnO NPs to green algae *Eremosphaera viridis*. Environ. Sci.: Nano 9, 393–405. https://doi.org/10.1039/D1EN00881A.

Yu, Q., Wang, Z., Wang, G., Peijnenburg, W.J.G.M., Vijver, M.G., 2022. Effects of natural organic matter on the joint toxicity and accumulation of Cu nanoparticles and ZnO nanoparticles in *Daphnia magna*. Environ. Pollut. 292, 118413. https://doi.org/10.1016/j.envpol.2021.118413.

Yu, R., Wu, J., Liu, M., Chen, L., Zhu, G., Lu, H., 2016a. Physiological and transcriptional responses of *Nitrosomonas europaea* to TiO_2 and ZnO nanoparticles and their mixtures. Environ. Sci. Pollut. Res. 23, 13023–13034. https://doi.org/10.1007/s11356-016-6469-8.

Yu, R., Wu, J., Liu, M., Zhu, G., Chen, L., Chang, Y., Lu, H., 2016b. Toxicity of binary mixtures of metal oxide nanoparticles to *Nitrosomonas europaea*. Chemosphere 153, 187–197. https://doi.org/10.1016/j.chemosphere.2016.03.065.

Yu, Y., Mo, W.Y., Luukkonen, T., 2021. Adsorption behaviour and interaction of organic micropollutants with nano and microplastics — A review. Sci. Total Environ. 797, 149140. https://doi.org/10.1016/j.scitotenv.2021.149140.

Zettler, E.R., Mincer, T.J., Amaral-Zettler, L.A., 2013. Life in the "plastisphere": Microbial communities on plastic marine debris. Environ. Sci. Technol. 47, 7137–7146. https://doi.org/10.1021/es401288x.

Zhai, X., Zhang, X.-H., Yu, M., 2023. Microbial colonization and degradation of marine microplastics in the plastisphere: A review. Front. Microbiol. 14, 1127308. https://doi.org/10.3389/fmicb.2023.1127308.

Zhai, Y., Hunting, E.R., Wouters, M., Peijnenburg, W.J.G.M., Vijver, M.G., 2016. Silver nanoparticles, ions, and shape governing soil microbial functional diversity: Nano shapes Micro. Front. Microbiol. 7, 1123. https://doi.org/10.3389/fmicb.2016.01123.

Zhang, F., Wang, Z., Peijnenburg, W.J.G.M., Vijver, M.G., 2022a. Review and prospects on the ecotoxicity of mixtures of nanoparticles and hybrid nanomaterials. Environ. Sci. Technol. 56, 15238–15250. https://doi.org/10.1021/acs.est.2c03333.

Zhang, F., Wang, Z., Vijver, M.G., Peijnenburg, W.J.G.M., 2022b. Theoretical investigation on the interactions of microplastics with a SARS-CoV-2 RNA fragment and their potential impacts on viral transport and exposure. Sci. Total Environ. 842, 156812. https://doi.org/10.1016/j.scitotenv.2022.156812.

Zhang, F., Wang, Z., Vijver, M.G., Peijnenburg, W.J.G.M., 2021a. Probing nano-QSAR to assess the interactions between carbon nanoparticles and a SARS-CoV-2 RNA fragment. Ecotoxicol. Environ. Saf. 219, 112357. https://doi.org/10.1016/j.ecoenv.2021.112357.

Zhang, F., Wang, Z., Vijver, M.G., Peijnenburg, W.J.G.M., 2021b. Prediction of the joint toxicity of multiple engineered nanoparticles: The integration of classic mixture models and *in silico* methods. Chem. Res. Toxicol. 34, 176–178. https://doi.org/10.1021/acs.chemrestox.0c00300.

Zhang, H., Ji, Z., Xia, T., Meng, H., Low-Kam, C., Liu, R., Pokhrel, S., Lin, S., Wang, X., Liao, Y.-P., Wang, M., Li, L., Rallo, R., Damoiseaux, R., Telesca, D., Mädler, L., Cohen, Y., Zink, J.I., Nel, A.E., 2012. Use of metal oxide nanoparticle band gap to

develop a predictive paradigm for oxidative stress and acute pulmonary inflammation. ACS Nano 6, 4349–4368. https://doi.org/10.1021/nn3010087.

Zhang, H., Shi, J., Su, Y., Li, W., Wilkinson, K.J., Xie, B., 2020. Acute toxicity evaluation of nanoparticles mixtures using luminescent bacteria. Environ. Monit. Assess. 192, 484. https://doi.org/10.1007/s10661-020-08444-6.

Zhang, J., Chen, H., He, H., Cheng, X., Ma, T., Hu, J., Yang, S., Li, S., Zhang, L., 2020. Adsorption behavior and mechanism of 9-nitroanthracene on typical microplastics in aqueous solutions. Chemosphere 245, 125628. https://doi.org/10.1016/j.chemosphere.2019.125628.

Zhang, J., Zhang, X., Zhou, Y., Han, Q., Wang, X., Song, C., Wang, S., Zhao, S., 2023. Occurrence, distribution and risk assessment of antibiotics at various aquaculture stages in typical aquaculture areas surrounding the Yellow Sea. J. Environ. Sci. 126, 621–632. https://doi.org/10.1016/j.jes.2022.01.024.

Zhang, K., Zheludev, I.N., Hagey, R.J., Haslecker, R., Hou, Y.J., Kretsch, R., Pintilie, G.D., Rangan, R., Kladwang, W., Li, S., Wu, M.T.-P., Pham, E.A., Bernardin-Souibgui, C., Baric, R.S., Sheahan, T.P., Glenn, J.S., Chiu, W., Das, R., D′Souza, V., 2021. Cryo-EM and antisense targeting of the 28-kDa frameshift stimulation element from the SARS-CoV-2 RNA genome. Nat. Struct. Mol. Biol. 28, 747–754. https://doi.org/10.1038/s41594-021-00653-y.

Zhang, Q., Liu, T., Liu, L., Fan, Y., Rao, W., Zheng, J., Qian, X., 2021. Distribution and sedimentation of microplastics in Taihu Lake. Sci. Total Environ. 795, 148745. https://doi.org/10.1016/j.scitotenv.2021.148745.

Zhang, Y., Zhang, X., Li, X., He, D., 2022. Interaction of microplastics and soil animals in agricultural ecosystems. Curr. Opin. Env. Sci.

Health 26, 100327. https://doi.org/10.1016/j.coesh.2022.100327.

Zhao, C., Shao, B., Yan, M., Liu, Z., Liang, Q., He, Q., Wu, T., Liu, Y., Pan, Y., Huang, J., Wang, J., Liang, J., Tang, L., 2021. Activation of peroxymonosulfate by biochar-based catalysts and applications in the degradation of organic contaminants: A review. Chem. Eng. J. 416, 128829. https://doi.org/10.1016/j.cej.2021.128829.

Zhao, C.Y., Zhang, H.X., Zhang, X.Y., Liu, M.C., Hu, Z.D., Fan, B.T., 2006. Application of support vector machine (SVM) for prediction toxic activity of different data sets. Toxicology 217, 105–119. https://doi.org/10.1016/j.tox.2005.08.019.

Zhao, J., Dai, Y., Wang, Z., Ren, W., Wei, Y., Cao, X., Xing, B., 2018. Toxicity of GO to freshwater algae in the presence of Al_2O_3 particles with different morphologies: Importance of heteroaggregation. Environ. Sci. Technol. 52, 13448–13456. https://doi.org/10.1021/acs.est.8b00815.

Zhao, L., Qi, Y., Luzzatto-Fegiz, P., Cui, Y., Zhu, Y., 2020. COVID-19: Effects of environmental conditions on the propagation of respiratory droplets. Nano Lett. 20, 7744–7750. https://doi.org/10.1021/acs.nanolett.0c03331.

Zhao, T., Tan, L., Han, X., Ma, X., Lin, K., Wang, J., 2023. Energy metabolism response induced by microplastic for marine dinoflagellate *Karenia mikimotoi*. Sci. Total Environ. 866, 161267. https://doi.org/10.1016/j.scitotenv.2022.161267.

Zhong, S., Lambeth, D.R., Igou, T.K., Chen, Y., 2022a. Enlarging applicability domain of quantitative structure–activity relationship models through uncertainty-based active learning. ACS EST Eng. 2, 1211–1220. https://doi.org/10.1021/acsestengg.1c00434.

Zhong, S., Zhang, Y., Zhang, H., 2022b. Machine learning-assisted

QSAR models on contaminant reactivity toward four oxidants: Combining small data sets and knowledge transfer. Environ. Sci. Technol. 56, 681–692. https://doi.org/10.1021/acs.est.1c04883.

Zhou, J., Zhang, H., Liu, J., Gong, L., Yang, X., Zuo, T., Zhou, Y., Wang, J., You, X., Jia, Q., Wang, L., 2023. Effects of Fe_3O_4 nanoparticles on anaerobic digestion enzymes and microbial community of sludge. Environ. Technol. 44, 68–81. https://doi.org/10.1080/ 09593330.2021.1963324.

Zhu, H., Fu, S., Zou, H., Su, Y., Zhang, Y., 2021. Effects of nanoplastics on microalgae and their trophic transfer along the food chain: Recent advances and perspectives. Environ. Sci. Process. Impacts 23, 1873–1883. https://doi.org/10.1039/ D1EM00438G.

Zhu, Z., Su, M., Ma, L., Ma, L., Liu, D., Wang, Z., 2013. Preparation of graphene oxide–silver nanoparticle nanohybrids with highly antibacterial capability. Talanta 117, 449–455. https://doi.org/ 10.1016/j.talanta.2013.09.017.