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

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Propositions

Accompanying the thesis

"Modelling the Interactions of Advanced Micro- and Nanoparticles with Novel Entities" *By* **Fan Zhang**

1. The nano-QSAR is a useful tool to investigate the impacts of nanomaterials on the novel coronavirus, and it has the advantages of preliminary screening of effective ENMs that will save valuable research time (Chapter 2).

2. Microplastics termed the 'plastisphere' are capable of regulating the behavior and fate of the SARS-CoV-2 RNA fragment in multiple environmental media (Chapter 3).

3. Antagonism is the predominant mode of interaction of multiple engineered nanoparticles towards a variety of different aquatic organisms (Chapter 4).

4. The key strategy to quantitatively predict the joint toxicity of emerging or untested/unknown mixtures of multiple ENPs is to integrate the classical mixture toxicology methods with computational toxicology approaches (Chapter 5).

5. The nano-QSAR models developed by machine learning methods can aid in the prediction of the ecotoxicity of mixtures of nanoparticles (Chapter 6).

6. The safe operating space of the planetary boundary of novel entities is exceeded since the annual production and releases are increasing at a pace that outstrips the global capacity for assessment and monitoring (Persson *et al.*, 2022).

7. Planetary boundaries are of direct concern to ecotoxicology as the boundary "novel entities" refer to the new forms of chemical, particulate, energy, or microbiological contaminants (de Souza Machado *et al.*, 2019).

8. Computational modeling approaches have emerged as low-cost alternatives, especially those used to develop quantitative structure-activity relationship (QSAR) models (Chung *et al.*, 2023).

9. Artificial intelligence and molecular simulation play key roles in transforming nanotoxicity data into critical information, i.e., constructing the quantitative nanostructure (physicochemical properties)–toxicity relationships, and elucidating the toxicity-related molecular mechanisms (Yan *et al.*, 2023).

10. "What we know is a drop, what we don't know is an ocean." (Isaac Newton).

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