

## Special Issue

# Molecular Computational Modelling in the Context of Safe and Sustainability-by-Design Strategy

### Message from the Guest Editor

The safe and sustainability-by-design strategy (SSbD) is one of the most important topics in the context of the European Green Deal. Chemicals Strategy for Sustainability Towards a Toxic-Free Environment, COM (2020) 66. The strategy of SbD identified a number of actions to reduce negative impacts on human health and the environment associated with chemicals, materials, products, and services commercialized or introduced onto the EU market. In particular, the ambition of the CSS is to phase out the most harmful substances and substitute, as far as possible, all other substances of concern, otherwise minimize their use and track them. The SSbD framework aims to support the design and development of safe and sustainable chemicals and materials with research and innovation activities. In this context this special issue is dedicated to the molecular computational modelling supporting SSbD strategy, which includes both physic-based (materials modeling and molecular study) and data-base (chemoinformatic design).

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### Guest Editor

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### Deadline for manuscript submissions

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## International Journal of Molecular Sciences

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