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Computational Design and Modeling of DNA Nanostructures and DNA Nanodevices

Guest Editor:

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Deadline for manuscript submissions:
closed (20 November 2021)

Message from the Guest Editor

Dear Colleagues,

The unique self-recognition properties of DNA, ruled by the strict Watson–Crick base pairing rules, make this molecule an ideal material for the creation of self-assembling, predesigned nanostructures, and nanodevices. In the thriving area of DNA nanotechnology, the computational design, modeling, and simulation of such structures are still one of the most addressed topics in the field.

This Special Issue aims to cover works describing novel methods or molecular simulation approaches applied to DNA nanostructures and nanodevices, with the aim to provide a more reliable structural and dynamic description of this class of structures.

The volume is open to innovative contributions involving aspects of the following topics:

Molecular simulation of DNA structures;
Molecular simulations of DNA self-assembly;
Modeling of DNA nanostructures and nanodevices;
Simulating the aggregation of DNA nanostructures with proteins;
QM/molecular mechanical (MM) methods for DNA nanostructures;
Design, optimization, and visualization of large DNA nanostructures;
Enhanced sampling techniques applied to DNA nanoswitches and nanodevices.

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Message from the Editor-in-Chief

As the world of science becomes ever more specialized, researchers may lose themselves in the deep forest of the ever increasing number of subfields being created. This open access journal Applied Sciences has been started to link these subfields, so researchers can cut through the forest and see the surrounding, or quite distant fields and subfields to help develop his/her own research even further with the aid of this multi-dimensional network.

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