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State-of-the-Art in Chemical Sensors Modelling and Theoretical Statements

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Message from the Collection Editors

The dramatic growth in the interest toward chemical sensors based on aptamers, chemical aptasensors, requires one to take stock of the situation, recollecting ideas and information about the state-of-the-art and possible developments. To complement experiments with appropriate modelling is the most effective way to speed up progress. Aptamers allow massive calculations, such as those necessary in molecular dynamics and density functional theory, to envision their structure and to predict the docking with the target or to design the best strategy for functionalization on an appropriate substrate. Aptamer extreme flexibility makes both structure prediction and the envision of binding scenarios very challenging. A satisfactory and complete description of novel modified aptamers performances, the role of modifications in increasing affinity require a sort of theoretical investigation yet to come. For aptasensors, some standard issues concerning the interpretation of dose-response, linear and dynamical regime, impedance and amperometric data, diffusion, charge transport and so on deserve attention and consolidation. Feasibility and proof of concept studies are also welcome.

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Topical Collection

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