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Modeling and Design of Polymeric Architectures for Chemical Sensing

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Summary

Detection of warfare agents, explosives and toxic industrial chemicals through the use of chemical sensing is gaining increasing importance. The development and fielding of chemical sensor devices for sensing with the desired sensitivity and the required specifity through Edisonian approaches involves arduous tasks of search of proper chemistries, nanostructures and physical-chemical property match for the sensory materials and chemicals to be sensed. If the strict constraints on selectivity/elimination of false positive signals, and strict constraints on sensitivity are placed, the search space for materials and materials structures has to be guided by the principles of physics, chemistry and engineering processing of the materials. For instance, without the physically based, computationally derived guiding principles, the most time consuming step for fielding a sensing device would be the choice and development of the sensory material system. We have applied multiphysics approaches to study the systems such as conjugated polymers, which can be used as amplifying fluorescence (AF) sensing of explosives. The high sensitivity and selectivity of AF Polymers is accomplished by carefully matching the physical/chemical/electronic/optical characteristics with the analytes and analyzing the possible effects with the potential false positives. Using ab initio quantum chemistry, Density Functional Theory (DFT), and Time Dependent DFT methods, molecular mechanics, molecular dynamics methods we study mechanical, physical, chemical properties, as well as electronic structure, absorption/emission spectra of polymers, analytes and complexes for developing the required design principles. Armed with the understanding and data generated on the polymer-target chemical interactions at the atomistic and nanostructure level we anticipate to develop a better engineering decision mechanism to shorten the time required to field the sensing capabilities and chemical sensors.

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