

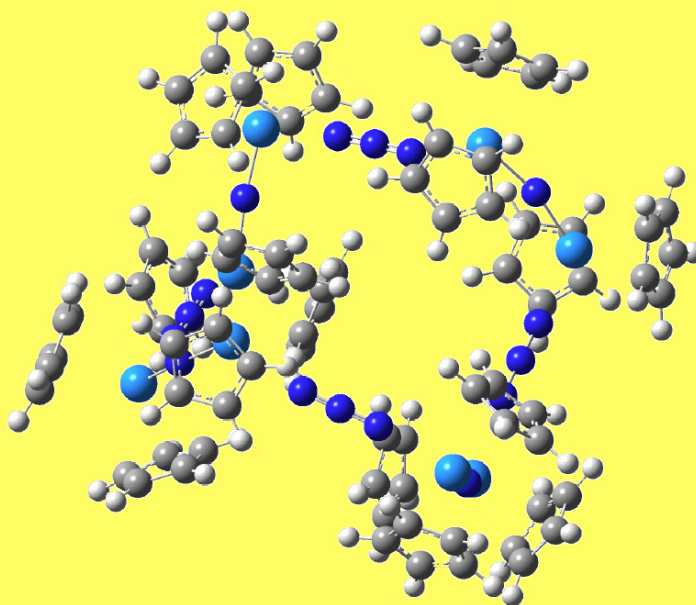


Modeling novel compounds related to renewable energies

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Quantum chemistry is a mature science that can be applied to the study of systems containing any atom in the periodic table. In this lecture I will discuss the state of the art of the field and how modeling can be employed to predict novel species that can be relevant to hydrogen storage. I will also describe our ongoing research on metapolynitrogen clusters. These compounds may represent a way to stabilize all-nitrogen molecules and may open new routes to the formation of high-energy density materials.



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