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First Principles Dynamics Beyond the Born-Oppenheimer Approximation[1]

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The dynamics of molecules in excited electronic states almost invariably involves breakdown of the Born-Oppenheimer approximation, necessitating treatment of quantum mechanical effects for both electrons and nuclei. The ab initio multiple spawning (AIMS) method has been developed in order to model molecular dynamics in excited states from first principles, solving both the electronic and nuclear Schrödinger equations "on the fly." We discuss some recent developments in the AIMS methodology and applications to photodamage in DNA bases. Theoretical results are compared directly to femtosecond spectroscopy experiments. Recent attempts to couple the AIMS approach with optimization algorithms to redesign fluorescent proteins will also be discussed, if time allows.

[1]In collaboration with Hanneli Hudock, Benjamin G. Levine, and Kristina Lamothe.