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First-Principles-Based Development of Kinetic Mechanisms in Chemically Active Light-Emitting Nonthermal Plasmas and Gases

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Recent progress in several related research areas such as first-principles electronic-structure calculations of atoms and diatomic molecules, theory of elementary processes, kinetics, and numerical engineering, and also continuing exponential growth in computational resources enhanced by recent advances in massively parallel computing have opened the possibility of directly designing kinetics mechanisms to describe chemical processes and light emission in such complex media as nonequilibrium plasmas and reacting gases. It is important that plasma and combustion kinetics can be described in the framework of this direct approach to a sufficiently high accuracy, which makes it an independent predictive research tool additional to experimental techniques. This paper is devoted to an overview of the key events in electronic structure theory, theory of elementary processes, kinetic theory, and computing engineering that provide a basis for this development. Two examples of the development of first-principles-based mechanisms devoted to mechanism of hydrocarbon fuel combustion at high temperatures and light emission in non-thermal glow discharge plasma of metal halides are discussed in detail with special attention paid to a comparison of the results obtained at every level of system description with the appropriate experimental data. Software tools that can be used in such multilevel theoretical works are discussed as well.