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Multilevel non-empirical approach to calculation of light emission properties of of chemically active non-equilibrium plasma B. POTAPKIN, S. ADAMSON, V. ASTAPENKO, I. CHERNYSHEVA, M. DEMINSKY, A. DEMURA, N. DYATKO, A. ELETSKII, A. KNIZHNIK, I. KOCHETOV, A. NAPARTOVICH, E. RYKOVA, S. UMANSKII, A. ZAITSEVSKII, Kintech, G. COTZAS, D. MIKHAEL, V. MIDHA, D. SMITH, T. SOMMERER, GE Global Research — A multi-level approach for calculation of the properties of non-equilibrium plasmas using first principles and theories of elementary processes is described in the paper. In the framework of this approach, unknown properties of molecules, ions and atoms (structure, energy curves, and transition dipole moments) are calculated using quantum-chemical methods. The calculation results are then used to determine emission probabilities, Frank-Condon factors of electronic-vibration transitions, cross sections for electron impact excitation, dissociation, dissociative recombination and attachment. Ion-molecular reactions are treated in terms of the statistical theory. The energy transfer processes involving electronically species are described through the asymptotic approach. The electron impact excitation cross sections for atoms and molecules are calculated using the modified Born approximation. The resulting kinetic state-to-state scheme is then used to compute the dependencies of the electron energy balance and the radiative emission efficiency as a function of the plasma parameters. As an example of this multilevel approach, the radiative emission properties of an Ar-InI DC glow discharge were calculated using the Chemical Workbench computational environment.

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