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Ab initio based calculation of emission properties of Ar-$AlCl_3$ glow discharge MAXIM DEMINSKY, BORIS POTAPKIN, STANISLAV UMANSKII, ALEXANDER ZAITSEVSKII, Kintech Lab, Moscow, Russia, DAVID SMITH, GE Global Reseach, Niskayuna,US, DARRYL MICHAEL, TIMOTHY SOMMERER, GE Global Reseach, Niskayuna, US — Emission properties of Ar-$AlCl_3$ DC glow discharge were calculated using "Chemical Workbench" VIBRAKIN code in frame work of quasi 1D model. Unknown properties of atoms and molecules were calculated from first principles. Potential energy curves of $Al_xCl_y^-$ negative ions were performed by approximate quadratic coupled cluster (AQCC) and SCF methods. Potential energy curves, transition dipole moments of neutral species Al_xCl_y were calculated based on many-body multipartitioning perturbation theory (MPPT). These data are used for evaluation of the cross sections of the electron impact dissociative attachment and vibrational excitation for $AlCl_3$ and fragments of its decomposition. The cross sections of the electron impact excitation of electronic states of atoms and molecules are evaluated in frame work modified Born approximation with taking into account electron exchange. Based on calculated properties of molecular ions, the rate parameters of thermal ion-molecular reactions of molecular ions conversion were calculated. The calculation results present dependencies of the electron energy balance and the emission efficiency as a function of the plasma parameters.

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