# A STUDY OF THE ELECTRONIC STRUCTURE OF PHENYLSILANES BY X-RAY EMISSION SPECTROSCOPY AND QUANTUM CHEMICAL CALCULATION METHODS

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The electronic structure of a series of phenylsilanes $Ph_{4-n}SiH_n$ ($n$ = 0-3) is studied by X-ray emission spectroscopy and quantum chemical calculations by the density functional theory method. Based on the calculations theoretical X-ray emission Si$K\beta_1$ spectra of phenylsilanes $Ph_{4-n}SiH_n$ ($n$ = 0-4) are constructed and their energy structure and shape turn out to be well consistent with experiment. The distribution of the electron density of states with different symmetry of Si, C, H atoms are also constructed. An analysis of the obtained X-ray fluorescent Si$K\beta_1$ spectra and the distribution of the electron density of states in $Ph_4Si$ and $Ph_3SiH$ compounds shows that their energy structure is mainly determined by a system of the energy levels of phenyl ligands weakly perturbed by interactions with valence AOs of silicon. In the energy structure of MOs of the $PhSiH_3$ compound, energy orbitals related to $t_2$ and $a_1$ levels of tetrahedral $SiH_4$ are mainly presented.

**Keywords:** electronic structure, phenylsilanes, X-ray emission spectroscopy, density functional theory.