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## The XPS structure and the peculiarities of the chemical bond nature in CeO<sub>2</sub>

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Cerium dioxide is known as a non-radioactive structural substitute of actinide oxides (UO<sub>2</sub> and PuO<sub>2</sub>). CeO<sub>2</sub>-based ceramics is suggested as an inert <sup>239</sup>Pu or <sup>235</sup>U bearing matrix for nuclear fuel, as well as a matrix for high-level waste disposal. CeO<sub>2</sub> is also used as an exhaust gas afterburning catalysts and in electronics.

X-ray photoelectron spectral structure of CeO<sub>2</sub> valence electrons in the binding energy range 0--50 eV was analyzed. The core-electron spectral structure parameters and relativistic discrete-variational calculation results for the CeO<sub>8</sub>12- (D<sub>4h</sub>) cluster reflecting cerium close environment were taken into account. Comparison of the valence and the core-electron spectral structures showed that formation of the inner (IVMO) and the outer (OVMO) valence molecular orbitals contributes to the spectral structure more than the many-body processes. The Ce 4f electrons were established to participate directly in the chemical bond formation in CeO<sub>2</sub> losing partially their f nature. They were found to be localized mostly within the outer valence band. The Ce 5p atomic orbitals were shown to participate in the formation of both the inner and the outer valence molecular orbitals. A most of part in the IVMO formation is taken by the filled Ce 5p<sub>1/2,3/2</sub> and O 2s atomic shells, while the Ce 5s electrons participate weakly in the chemical bond formation. The composition and the sequent order of the molecular orbitals in the binding energy range 0--50 eV was established. A quantitative scheme of the molecular orbitals for CeO<sub>2</sub> was built. This scheme is fundamental also for the interpretation of other X-ray spectra of CeO<sub>2</sub>. Evaluations yielded that the IVMO electrons weaken by 37 % the chemical bond formed by the OVMO electrons.

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