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Ionicity and inhomogeneous charge distribution by polarons and excitons in HfO₂ ALD films

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HfO₂ ALD films are studied using resonant photoelectron spectroscopy (resPES). We deduce that the electronic structure of HfO₂ is dominated by coexisting electron and ionic states/bonds caused by charge polarization and self-trapping phenomena of the valence charges. They stabilize intrinsic electronic defect states – such as polarons and excitons - which have different degree of spatial localization and electronic correlation [1, 2].

Their relative abundance can be determined by the ionicity factor f_i and its value can be derived from the resPES data as well. Both, ionicity and intrinsic electronic defects are used to explain the optical, electrical and transport properties.

- [1] D. Schmeißer, M. Kot, S. Alberton Corrêa, C. Das, K. Henkel, in K. Wandelt (Ed.): Encyclopedia of Interfacial Chemistry: Surface Science and Electrochemistry, Elsevier, Oxford, 2018, vol. 3.1, pp 162-171.
- [2] K. Henkel, M. Kot, M. Richter, M. Tallarida, D. Schmeißer, in K. Wandelt (Ed.): Encyclopedia of Interfacial Chemistry: Surface Science and Electrochemistry, Elsevier, Oxford, 2018, vol. 3.1, pp 18-26.