The electronic structure library in the search for new functional materials

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Abstract. We have used a Full-Potential Linear Muffin-Tin Orbital model from the Density Functional Theory together with information from the Inorganic Crystal Structure Database to perform automatized Electronic Structure calculations of roughly 22,000 inorganic compounds. We describe the methodology behind the automatized calculations and present the results generated, we show how to construct selection criteria and how these can be used to identify new functional materials in the database. We finally propose a feasible small number of possible new detector materials for ionizing radiation, of which some were synthesized and confirmed experimentally.