Machine learning driven computational platform for designing high functional materials toward surface reactions

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Using first-principles density functional theory (DFT) calculations and ab-initio molecular dynamic (AIMD) simulations we establish big data for materials properties toward surface chemical/electrochemical/optical reactions. With careful analysis the database using neural network and machine learning approach we identify key descriptors for catalytic activity for proton electrolyte membrane fuel cells, resolution of biosensors utilizing photo spectrum, and capacity of a counteragent for hazardous chemicals. The descriptor can be useful for a design principles for even further optimizing the materials and screen promising candidates.