Machine learning accelerated optimization of cluster and surface structures

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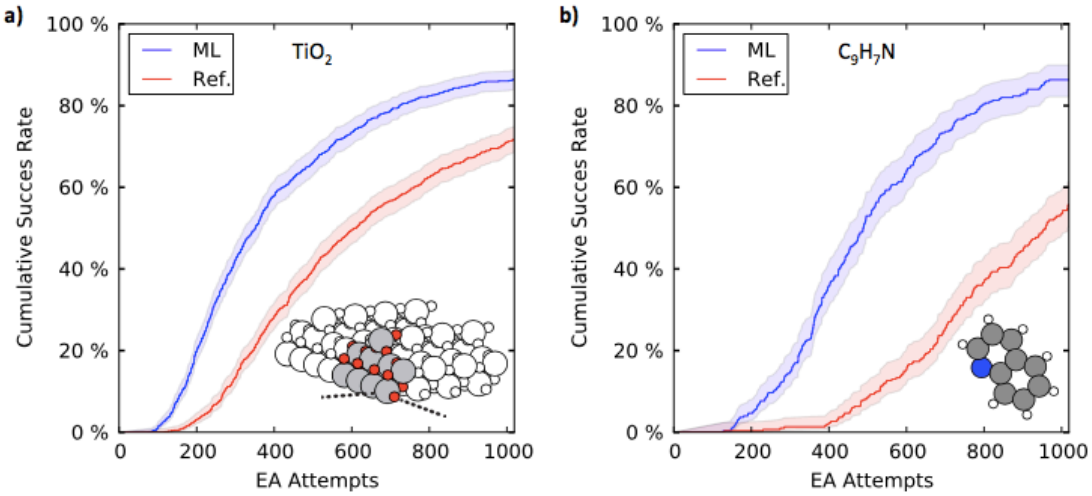
A number of search methods based on basin hopping or evolutionary algorithms are routinely used to identify, e.g. in a density functional theory framework, the most optimal cluster and surface structures for various inorganic compounds. In this talk, it is shown, how simple machine learning models, when introduced in the search methodologies, may accelerate such searches. The machine learning models include unsupervised and supervised models, such as clustering[1], kernel enabled regression methods[2,3], and artificial neural networks[4,5]. Common the methods is a need for a proper representation of the compound structures and a discussion of different representations is hence taken, in particular with a view at the amount of data being available.



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