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Chapter 17 - Structure prediction using reactivity descriptors

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Abstract

This chapter reviews different approaches proposed to use a local descriptor, the Fukui function, and a global descriptor, the chemical potential, to guide the exploration of the potential energy surface of clusters and molecules. Different proposals use assembly blocks, molecules, or clusters, whose combination produces the stoichiometry of the system under study. The choice of a Fukui function lies on its relationship with the interaction energy of the assembly units under perturbative theory. Several applications are shown, where the global minima and best minima of several benchmark systems are successfully identified.

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