CARE an automated reaction network for heterogeneous catalysis

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We have created a machinery able to carry out the quantification of reactivity fully automatize. CARE employs a rule based generator, a cheap energy evaluator based on a graph neural network considering uncertainty quantification and finally a microkinetic module. Our code is able to run even for very demanding reaction networks, such as the Fischer-Tropsch synthesis up to C6 products, accounting for 370k elementary steps.