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over pt and pt re catalysts the values of the reaction rates and reaction orders predicted by the model are in agreement with the'
'*the coupling of experiments with density functional theory*

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June 1st, 2020 - in the 1970s density functional theory dft was borrowed from physics and adapted to chemistry by a handful of visionaries now chemical dft is a diverse and rapidly growing field its progress fueled by numerous developing practical descriptors that make dft as useful as it is vast

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degree rotation h1 h 2 of the other given that the rotation barrier between the two conformers i s small less than 1 kcal mol depending on the level
of th e ory and basis set it is conceivable that qmd simul a"**perspectives on the density functional theory of chemical**

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June 5th, 2020 - stefan grimme university of bonn germany develops methods for theoretical chemistry here he talks to catharina goedecke for chemviews magazine about his research in particular about the popular dft d3 method used to account for dispersion interactions in density functional theory dft calculations grimme won the prestigious gottfried wilhelm leibniz prize the highest honor awarded in'

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May 19th, 2020 - the fukui function f was proposed as a tool for deducing the relative reactivity of different positions in a molecule by parr and yang in 1984 herein we sketch the theory of the fukui function with special emphasis on its logical motivation interpretation qualitative characteristics and practical putation we conclude with some words about the fukui function s extensions"

**'study of the reactivity of 100 felodipine surface model
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