chemisch
physikalische
gesellschaft

Gegründet im Jahre 1869 von H. Hlasiwetz, J. Loschmidt, J. Petzval und J. Stefan

EINLADUNG

zum

virtuellen Vortrag

von

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Center for Molecular Biosciences

Reaction Mechanisms and Reactivity of Complex Systems Uncovered by Computational Chemistry

am

Dienstag, 12. Jänner 2021, um 17:30 Uhr

Einladung und Zugangsdaten zum Online-Vortrag wurden an die CPG-Mitglieder versandt.
Für weitere Interessierte sind die Zugangsdaten auf Anfrage erhältlich, bitte E-Mail an
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Abstract

Computational modelling in chemistry and materials sciences has significantly gained importance over the last three decades. It has undoubtedly contributed to the understanding of reaction mechanisms and reactivity at an atomistic level and is a key element for the design of new molecules or materials.

I will showcase how quantum chemical and molecular mechanical methodologies can be used to rigorously characterize complex systems at examples related to materials science and catalysis. I will also address some in the challenges in state-of-the-art quantum chemical modelling of (homogeneous) catalysis and how to overcome them to arrive at a more reliable description – a prerequisite for predictive modelling.