



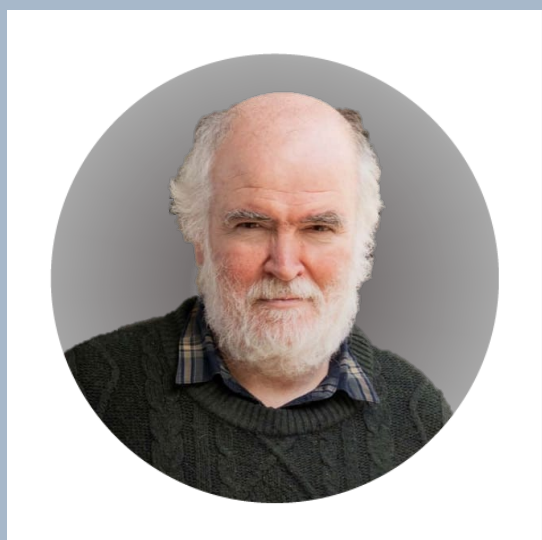
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**From computational
homogeneous catalysis
to computational
mechanochemistry**

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From computational homogeneous catalysis to computational mechanochemistry

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Computational homogeneous catalysis has made enormous progress in the last decades. The improvement of theoretical algorithms and the increase of computer power have led to an improved understanding of a variety of processes, and to the use of calculation as a tool for reaction optimization. This has been a major line of research in our group, and we have contributed with the study of a variety of processes. We will briefly review our contributions in this concern.

The tools of computational homogeneous catalysis include density functional theory (DFT) and, in recent years, microkinetic modeling (MKM). These same tools can be applied also to other fields of chemistry that have been less explored. Following this idea, we have entered in recent years areas as diverse as ball-milling mechanochemistry and organic electrosynthesis. Some of the applications in mechanochemistry will be also discussed.