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DFT and Catalysis

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Message from the Guest Editor

Density functional theory (DFT) calculations have been a powerful research tool for decades. Particularly, the knowledge and theory obtained from DFT-based calculations have effectively refined our understanding of fundamental surface science, catalysis, and materials science. This Special Issue covers the fundamentals of DFT and related computational methods applied in surface chemistry and catalysis, especially in the field of heterogeneous and electrochemical catalysis. The Guest Editor hopes that the topics covered in this Special Issue will convey the expanding potential of density functional theory (DFT) calculations and will be of interest to those working in the field.I look forward to receiving original contributions or review papers.