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Guiding the Discovery of Single-Atom Catalysts with Quantum Chemical Simulations

Single Atom Catalysts (SACs) are an emerging frontier in the field.1 Computational chemistry offers a valid framework to access the atomistic details of catalytic processes, to rationalize or even predict novel systems. The state-of-the-art approach to model and to rationalize these objects takes insight from heterogeneous catalysis.2 In this presentation I will discuss the key ingredients to guide the discovery of SACs. SACs can be considered "solid-state" analogues of coordination chemistry compounds,3 which undergo a very different reactivity from solid surfaces. We show that the same can occur on SACs and this has relevant implications to the predictions.4,5 In addition, we propose an approach to predict the stability of SACs under experimental working conditions.6 We show evidence suggesting that self-interaction corrected schemes should be adopted due to the atomic-like character of SACs.7 Density functional theory numerical simulations demonstrate that these ingredients must be considered to provide reliable predictions about the activity of SACs.8 These studies provide an example of the important analogies between the chemistry of SACs and that of coordination compounds. The results underline the key ingredients to be accounted when attempting to provide predictions with computational frameworks, and aspect of dramatic importance to guide the discovery of new SACs.

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Primary author(s) : Dr. DI LIBERTO, Giovanni (University of Milan-Bicocca); Prof. PACCHIONI, Gianfranco (University of Milan-Bicocca)

Presenter(s) : Dr. DI LIBERTO, Giovanni (University of Milan-Bicocca)