Machine learning potentials to bridge the gap between theory and experiments in zeolite catalysis

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Zeolites are a class of microporous aluminosilicates widely used as catalysts in the chemical industry. Not only are they the workhorse of traditional oil refinery, but they are nowadays also widely used in sustainable processes such as biomass conversion and methanol-to-hydrocarbons, among others[1]. A fundamental understanding of their working mechanism is essential to improve their catalytic function, with major economic and environmental benefits. This is complicated by the intricate nature of zeolites[2]. They present a variety of poorly understood active sites, strong and reactive material-adsorbate interactions and they can undergo extensive spatiotemporal changes such as coking and mesopores formation.
Molecular simulations are essential to understand the working principles of catalytic processes and materials at the nanoscale, with the overarching goal of guiding, complementing and explaining the experiment. Thus far, the high computational cost of first-principles methods (most commonly density functional theory, DFT) did not easily allow to reach the simulation length- and timescales needed to investigate realistic processes at operating conditions[3]. Herein, we present our recent efforts in exploiting machine learning potentials (MLPs) to model realistic materials and catalytic processes[4,5]. MLPs can be orders of magnitude cheaper than the first-principles methodology used to train them, while retaining analogous accuracy. We showcase how MLPs can be used to model intricate zeolite-catalyzed reactions accessing accuracies, length- and timescales thus far precluded to molecular simulations, gradually bridging the gap between theory and experiments.

References

1. Ennaert, T. et al. *Chem. Soc. Rev.* **2016**, 45, 584-611.
2. Chizallet, C. *ACS Catal.* **2020**, 10, 5579-5601.
3. Van Speybroeck, V. et al. *ACS Catal.* **2023**, 13, 11455-11493.
4. Bocus, M. et al. *Nat. Comm.* **2023**, 14, 1008.
5. Vandenhaute, S. et al. *npj Comput. Mater.* **2023**, 9, 1-8.