

# Artificial intelligence for chemistry

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Artificial Intelligence (AI) has fully entered our everyday lives. It is used to power search engines, advertising, text translation, social networks and to assist medical diagnosis. Why has AI made such a boom in the last years? The massive increase in computing power, coupled to advances in machine learning algorithms and to the generation and storage of vast amounts of data on the internet are the main factors explaining this boom.

Without any doubt, chemistry will also benefit from this boom,<sup>1</sup> but R&D efforts in AI applied to chemistry have barely started.

In this presentation, we will present selected examples of successful application of AI to chemical problems (development of advanced materials, molecule retrosynthesis, discovery of new compounds). We will also discuss the opportunities and challenges faced by chemists who integrate AI in their research.

- (1) Butler, K. T.; Davies, D. W.; Cartwright, H.; Isayev, O.; Walsh, A. *Nature* **2018**, 559, 547–555.