Practical Introduction to Artificial Intelligence in
Quantum Chemistry

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In this pedagogical lecture, I will give an introduction to the use of artificial intelligence/machine learning for improving the performance and accuracy of quantum chemical simulations. This introduction is practical and based on our extensive experience in research and teaching (see, e.g., the recent book [Quantum Chemistry in the Age of Machine Learning](https://www.elsevier.com/books/Quantum%20Chemistry%20in%20the%20Age%20of%20Machine%20Learning/9780323900492), edited by P. O. Dral, Elsevier, 2023, and our group’s website [dr-dral.com](http://dr-dral.com)). I will also give concrete examples of how to perform simulations with our general-purpose package for atomistic machine learning simulations MLatom ([MLatom.com](http://MLatom.com)) using the XACS cloud computing service ([XACScloud.com](https://XACScloud.com)).



Figure 1. Machine learning greatly speeds up quantum chemical simulations, a figure from P. O. Dral, M. Barbatti. *Nat. Rev. Chem.* **2021,** *5*, 388–405.