Perspective on drug design on quantum computers

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The promised industrial applications of quantum computers often rest on their anticipated ability to perform accurate, efficient quantum chemical calculations. Computational drug discovery relies on accurate predictions of how candidate drugs interact with their targets in a cellular environment involving several thousands of atoms at finite temperatures. Although quantum computers are still far from being used as daily tools in the pharmaceutical industry, in this talk, I will explore the challenges and opportunities of applying quantum computers to drug design. Based on the findings from past and present projects by the Quantum Lab at Boehringer Ingelheim, I'll discuss the impact on industrial research and identify the substantial further developments needed to reach industrial relevance.