

**Pressemitteilung****Technische Universität Berlin****Stefanie Terp**

10.09.2020

<http://idw-online.de/de/news753929>Forschungsprojekte  
Informationstechnik, Medizin  
überregional**Using Machine Learning to Combat the Coronavirus****Research project developed by TU Berlin and the University of Luxembourg receives funding of 125,000 US dollars from Google.org**

Joint press release of the University of Luxembourg and Technische Universität Berlin

Using Machine Learning to Combat the Coronavirus

Research project developed by TU Berlin and the University of Luxembourg receives funding of 125,000 US dollars from Google.org

The intensive binding of the SARS-CoV-2 spike protein on human host cells appears to be a significant factor in the virus's high infectiousness. A joint team of researchers from TU Berlin and the University of Luxembourg is exploring why this spike protein is able to bind so much more effectively than other coronaviruses. Google.org is funding the research with 125,000 US dollars. Globally, Google.org funds 31 coronavirus research projects.

The project is led by Dr. Grégoire Montavon from TU Berlin's Chair of Machine Learning of Professor Dr. Klaus-Robert Müller and Professor Alexandre Tkatchenko of the University of Luxembourg. Using an approach which combines quantum mechanics and machine learning, the project seeks to gain a deeper understanding of the binding behavior of the novel coronavirus (SARS-CoV-2).

Exact simulation of the molecular dynamics of the spike protein

The researchers are analyzing the mechanism which accounts for the unusually high binding affinity displayed by the SARS-CoV-2 spike protein regarding ACE2 human host cell receptors: Discovering this process would represent an important first step towards the future development of treatments for the coronavirus. Using precise, long-term simulations of the molecular dynamics of the spike protein and the human receptor, the researchers aim to gain a better understanding of how they interact. Simulating molecular dynamics reveals the movement caused by the interaction of single atoms within an atom system over time. Special machine learning processes are to be developed for the enormously complex calculations involved. "Examining the adhesion mechanism of SARS-CoV-2 presents us with a host of new challenges: The systems contain hundreds of thousands of atoms and a wide range of possible adhesion scenarios has to be taken into account. These challenges require a truly interdisciplinary approach," says Professor Dr. Alexandre Tkatchenko of the University of Luxembourg.

"We are delighted to be receiving this funding and support for our fundamental research," adds Grégoire Montavon. "Upon completion of the project, we will be publishing our findings for the entire scientific community."

Further information is available from:



Dr. Grégoire Montavon  
TU Berlin  
Chair of Machine Learning  
Phone: 030 314-78755  
Email: [gregoire.montavon@tu-berlin.de](mailto:gregoire.montavon@tu-berlin.de)

