Molecular simulations are capable of reproducing and predicting the behavior of real systems using a simplified model. Over the past 70 years, thanks to the rapid development of computers, this method has become an important part of various scientific fields. Thanks to their speed and low cost, molecular simulations can work hand in hand with a real experiment and in some cases even replace it. The didactics of this progressive method are in its beginnings at the Faculty of Science of Charles University, and its teaching is limited to master's and higher studies. In this work, we created and tested a task for physical chemistry laboratory, which can serve as a first introduction to molecular simulations for undergraduate chemistry students. The task, written in the interactive Jupyter Notebook environment, was designed based on modern pedagogical approaches of inquiry based learning, supplemented by a high level of scaffolding due to the complexity of the teaching content. The choice of simulating the model of supercritical argon described by the Lennard-Jones potential was based on the requirement for conceptual simplicity and the possibility of connection with already known concepts. Testing of the task on 12 students made it possible to create a time schedule, correct errors, identify the most common problems, and propose suggestions for improvement. We would be glad, to have the task included as a regular part of the physical chemistry laboratory or in the course of physical chemistry on the Faculty of Sciences at the Charles University.