

Prague 18.5. 2022

Subject: Statement of the PhD mentor of A. Gallardo

To Whom It May Concern,

Aurelio Gallardo began his doctoral studies in 2017 at the Institute of Physics of the Czech Academy of Sciences. In a short time, he was able to master the necessary theoretical foundations of electronic structure calculation as well as scanning probe microscopy. He also got acquainted with the issue of molecules on surface and weak intermolecular interactions. He used this knowledge to study the halogen bonds between molecules on the surfaces of solids and the possibility of their imaging using scanning microscopy. He also learned QM/MM calculations, which he later applied to the simulation of chemical reactions on solid surfaces. The simulations enabled to obtain a detailed picture of experimentally observed chemical transformation.

He actively participated in the development of a program to simulate scanning microscopy images. The simulations performed by them significantly helped to optimize the experimental measurements, which make it possible to display the anisotropic distribution of the atomic charge.

During his thesis, he learned to communicate with experimental fellows and to explain them his theoretical results in an understandable form. He actively participated in the scientific activities of the Nanosurf laboratory at the Institute of Physics. Recently, he also participated in the mentoring of younger PhD students, to whom he transfers his experience with theoretical simulations.

He presented his results at a number of international conferences, where he demonstrated good presentation skills. During his doctoral studies, he demonstrated the ability of independent scientific thinking. These qualities give good preconditions for his future independent scientific career. Thus, I fully recommend the award of a PhD degree.

Dr Pavel Jelinek  
Nanosurf Lab  
Institute of Physics of the CAS  
Cukrovarnicka 10  
Prague 6  
CZ 162 00  
Czech Republic  
tel: +420 220 318 430  
fax: +420 233 318 468  
[email: jelinekp@fzu.cz](mailto:jelinekp@fzu.cz)