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**APPLICATION FOR THE DISTINCTION OF A DOCTORAL DISSERTATION**

Author: Karol Baran, MSc Eng.
Title: *Few-shot machine learning for multimolecular systems modeling*

The scientific merit of the doctoral dissertation by Karol Baran, MSc Eng., justifies an application for its distinction. I base this application on two grounds, relating to the quality of the results obtained and to their practical significance.

First, the solutions developed by the Candidate for modeling the properties of ionic liquids are markedly superior to the approaches used to date, which is unambiguously confirmed by the statistical parameters obtained. Introducing fractional free volume as a molecular descriptor raised the coefficient of determination of models predicting carbon dioxide solubility from 0.738 to 0.833 on the test set. A systematic resolution of how bimolecular systems should be represented in graph neural networks yielded models that were not only more accurate but also the most reproducible among the variants compared. The greatest significance, however, lies in demonstrating the effectiveness of the Candidate's own modifications of meta-learning algorithms for adaptation sets comprising only a few to a dozen or so compounds, that is, in a regime in which methods hitherto regarded as standard fail completely. The proposed TSA-Reptile algorithm improved the quality of predictions for systems distant from the training data, for which the standard meta-learning approach proved inadequate.

Second, the results obtained carry clear implementation potential. The models developed address problems of genuine technological relevance, including carbon dioxide capture, the isolation of lignin from biomass, and the safety assessment of the solvents employed. They can be applied directly to the screening of ionic liquids prior to the experimental stage. At the same time, the algorithmic modifications proposed are independent of the field of application. Ionic liquids serve in the dissertation as a demanding model system, while the solutions developed can be transferred to other areas in which the amount of available measurement data remains limited.

For the reasons set out above, I hereby apply for the distinction of the reviewed doctoral dissertation.

Signature Not Verified
Dokument podpisany przez Krzesimir Ciura
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