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Re: evaluation of thesis of Karol Baran: "Few-shot machine learning for multimolecular systems modeling" submitted to Gdańsk University of Technology

Dear Faculty,

I highly recommend the doctoral dissertation of Mr Karol Baran for distinction. This work represents an outstanding, pioneering contribution to the field of chemoinformatics, as it transfers "domain adaptation" methods from machine learning to the analysis of multimolecular chemical systems which is a field characterized by a scarcity of data.

Rather than simply applying existing machine learning algorithms, Karol Baran developed and proposed novel methodological improvements:

1. The candidate convincingly demonstrated that the separate optimization of ion geometries integrated into a unified graph yields the best predictive performance for graph neural networks (GNNs).
2. Attentive Model-Agnostic Meta-Learning (Att-MAML)—an extension of the standard MAML algorithm that incorporates an auxiliary scaling layer to adjust the importance of latent features when predicting toxicity in few-shot learning scenarios, including cases where the dataset contains as few as four samples.
3. Task Similarity-Aware Reptile (TSA-Reptile)—a method that utilizes task similarity assessment (based on Tanimoto chemical similarity) to dynamically scale the loss function, thereby outperforming standard meta-learning methods when addressing highly unique tasks.
4. Baran developed an innovative two-stage protocol involving the pre-training of a meta-learning model on thermodynamic modeling data (COSMO-RS), followed by fine-tuning on experimental values; this approach significantly mitigates the data scarcity problem encountered in the development of "green" solvents.

The methodologies and models developed in this dissertation can find direct practical application in key areas of green chemistry—such as carbon capture and sequestration. This is achieved through the creation of robust models for assessing and interpreting CO_2 sorption processes in specially designed ionic liquids, the development of interpretable machine learning algorithms to optimize the extraction of high-quality lignin from herbaceous biomass, and the facilitation of rapid, cost-effective screening for hazardous chemicals.

Thus, Karol Baran's dissertation demonstrates a rare combination of deep chemical intuition, high competence in computer science, and rigorous statistical validation. For these reasons, the work stands as an exemplary piece of scientific research and fully merits the highest grade.

Sincerely,

Igor V. Tetko
Tuesday, 25 August 2026, Munich