Auto-CheML software

User License Agreements

Please complete this form, scan and email it to Prof. Jing Ma via majing@nju.edu.cn (Dated: January 12th, 2025)

All requestors for Auto-CheML MUST agree to the following agreements:

1. I will not use this software for any commercial use.

dataset on all of your group's computer resources.

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- 2. I will not redistribute a copy of this software to a third party. Instead, I will refer any requests for copies of the software to you at Nanjing University.
- 3. Publications in which the software is used should cite Auto-CheML as:

Jiawei Chen, Yuming Gu, Qin Zhu, Yating Gu, Xinyi Liang, Jing Ma, Automated Machine Learning of Interfacial Interaction Descriptors and Energies in Metal-Catalyzed N₂ and CO₂ Reduction Reactions.

4. Anyone in your research group is covered by the license and may share your copy of this

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